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THIRUVALLUVAR UNIVERSITY

SERKKADU, VELLORE – 632 115

DEPARTMENT OF CHEMISTRY

MASTER OF SCIENCE IN CHEMISTRY

[Under Choice Based Credit System (CBCS)]

w.e.f the academic year 2018-19

SYLLABUS AND REGULATIONS

FOR UNIVERSITY DEPARTMENT

ABOUT THE DEPARTMENT

The department of chemistry was established in 2002 as post-graduate and research department. The full fledged department was started during academic year 2010-11. The department is offering the M.Sc., M.Phil. and Ph.D courses. The department consists of 6 faculty members, 1 administrative staff, 32 research scholars and 52 PG students. The faculty members have been working on the modern and thrust areas in chemistry with financial support from various national funding agencies such as DST, DRDO, BRNS, UGC etc., and continued to publish quality research papers in both national and international journals.

VISION AND MISSION

Statement of Vision

Chemistry provides immense scope for study, research andgainful employment in various sectors. The Department of Chemistry of Thiruvalluvar University is determined to educate and graduate rural students. The department is committed to prepare, compete in and contribute to the needs of modern chemical science based industries and academia. To achieve this vision, the department is dedicated to provide a course of study for post-graduate in chemistry which combines curriculum and research oriented project that are high-quality, innovative and intellectually challenging.

Statement of Mission

The mission of the Department of Chemistry of Thiruvalluvar University is to advance the chemical sciences through the education of post-graduate students in rural society by providing them with quality classroom learning and research opportunities. The department is committed to impart a high standard for excellence in all branches of chemistry by innovative and dedicated teaching at post-graduate level to produce students with good knowledge in chemistry.

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THIRUVALLUVAR UNIVERSITY

Department of Chemistry

M.Sc., Chemistry (University Department)
UNDER CBCS (With effect from 2018-19)

The course of study and scheme of examinations

1. **TITLE:** M.Sc., Chemistry
2. **YEAR OF IMPLIMENTATION:** July 2018 onwards
3. **COURSE DETAILS:**

Total No. of Semesters	– 04 (Two semesters per year)
No. of theory papers per semester	– 04
Total No. of theory papers	– 16
No. of practical courses per semester	– 03 (upto III semester)
Total No. of Practicals	– 09
Project	– IV semester

Total Marks for M.Sc. Degree

Theory	-1600 marks
Practicals	- 900 marks
Project	- 100 marks
Total	**-2600 marks**

4. PREAMBLE OF THE SYLLABUS:

Master of Science (M.Sc.) in Chemistry is a post graduation course of Thiruvalluvar University. The curriculum is prepared by following the prospectus of various national and international universities. The board of studies revised the syllabus of M.Sc.,Chemistry in 2018 and the new revised syllabus covers broad area of fundamental aspects in modern chemistry.

The syllabi are all set to meet the standard of CSIR-UGC-NET,GATE and SLET examinations. The credit system to be implemented through this curriculum would allow students to develop a strong footing in the fundamentals and specialize in the disciplines of his/her liking and abilities. The students pursuing this course would have to develop in-depth understanding of various aspects of chemistry. The conceptual understanding, development of experimental skills, designing and implementation of novel synthetic methods, developing the aptitude for academic and professional skills, acquiring basic concepts for structural elucidation with hyphenated techniques, understanding the fundamental biological processes and rationale towards computer. The project introduced in the curriculum will motivate the students to pursue the research and find a job in reputed pharmaceutical and other industries including abroad.

5. REQUIREMENT TO APPEAR FOR THE EXAMINATION

(i) Minimum 75% attendance required for both theory and practical examinations.
(ii) Attendance of less than 75% but 65% and above has to pay the condonation fee prescribed by the university.
(iii) Attendance less than 65% but 55% and above has to compensate the shortage of attendance in the subsequent semester (in the next year).

(iv) Attendance less that 55% has to rejoin / redo the semester.
(v) In the case of married woman, the minimum attendance should not be less than 55%.

6. PATTERN OF EXAMINATION

Evaluation of Students:
1. All Semester examinations both theory and practical will be of 100 marks each.

2. Student has to obtain 50% marks in all the examinations (both theory and practicals).

7. FEE STRUCTURE: As per Thiruvalluvar University norms

8. ELGIBILITY FOR ADMISSION

A candidate who has passed the B.Sc., degree examination with Chemistry as the main subject of study of this university or an examination of any other university accepted by the syndicate as equivalent thereto shall be eligible for admission to the M.Sc., degree in chemistry in the university department.

9. MEDIUM OF INSTRUCTION: English.

10. SCHEME OF EXAMINATION

• The semester examination will be conducted at the end of each semester (Both theory & practical examination), for odd semesters in the month of November/December; for even semester in April/May. All theory examination is conducted for 3 hours irrespective of total marks. However, duration of practical examinations is 6 hours.
• **Theory paper** will be of 75 marks each for university examination and 25 marks for internal evaluation.
  - **Theory question pattern**

Section-A	10×2	= 20 marks (50 words; no choice)
Section-B	5×5	= 25 marks (200 words; Either or type)
Section-C	3×10	= 30 marks (500 words; 3 out of 5)
	Total	**= 75 marks**

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- **Internal Assessment**

Test	: 10 marks (best 2 out of 3)
Assignment	: 10 Marks
Seminar	: 05 Marks
Total	**: 25 marks**

There shall be tutorial / practical / surprise test / home assignment / referencing of research papers / seminar / industrial visit / training course as a part of internal assessment in each semester. The students are supposed to attend all the tests. The students should note that re-test will not be given to the student absent for the test/s.

- **Practical examination** will be of 75 marks each for university examination and 25 marks for internal evaluation.

Distribution of marks for practical examinations

University Examination Experiment : 75 Marks

Procedure	: 5 marks
Experiment	: 30 marks
Interpretation	: 10 marks
Result	: 10marks)
Practical viva-voce	: 10 marks
Record	: 10 Marks
Total	**: 75 marks**

Practical Internal Assessment

Number of Experiments	: 10 marks
Performance	: 10 Marks
Test	: 5 Marks
Total	**: 25 marks**

Passing Minimum in practical examinations

IA	: 12 Marks (50 %)
UE	: 38 Marks (50 %)
Total	**: 50 Marks**

All the practical examinations will be conducted for 6 hours only i.e. 10 AM – 4PM by both the internal examiners.

- For the project report

Report	: 75 marks
Viva-voce	: 25 marks
Total	**: 100 Marks**

Distribution of marks for project report (Total of 100 marks)

Project will be evaluated by the concerned project guide along with a member nominated by the Head of the Department.

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Assessment will be done by the departmental committee every month. Evaluation will be on the basis of monthly progress of project work, progress report, referencing, oral, results and documentation.

Project - 75 marks
(Dissertation Format – 10 marks; Scope of the research problem – 20 marks; Methodology – 20 marks; Analysis – 10 marks, Results and findings-15 marks)

Viva-Voce examination – 25 marks
(Presentation – 10 marks; subject knowledge – 10 marks; Interaction – 5 marks)

11. Question papers will be set in the view of the entire syllabus and preferably covering each unit of the syllabus.

12. STANDARD OF PASSING
A candidate should get not less than 50% in the university examination, compulsorily, in all papers, including practicals. Also, the candidate who secures not less than 50% marks in the UE and IA examinations put together in any theory paper/practical shall be declared to have successfully passed the examination.

- Internal marks will not change. Student cannot repeat internal assessment. If student misses internal assessment examination, s/he will have to score passing minimum in the external examinations only.

Illustration: Theory – Internal Assessment -12 marks and University Examination-38 marks

OR

Internal Assessment-0 marks and University Examinaiton-50 marks.

- There shall be revaluation of answer script of end semester examination, but not of internal assessment papers.
- Internal assessment answer scripts may be shown to the concerned student but not end semester answer script.

❖ A candidate shall be declared to have passed the whole examination if the candidate passes in all theory and practical by earning 90 credits in core and elective subjects.

13. TRANSITORY PROVISION
This curriculum is valid for three years only (2018-19 to 2020-21), as per UGC norms. Hence, candidates who have undergone M.Sc., Chemistry course in the University department will be permitted to re-appear for next two consecutive years only. After that, he/she has to re-appear for the examinations under new curriculum, regulations, which are in force at that time.

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THIRUVALLUVAR UNIVERSITY
DEPARTMENT OF CHEMISTRY
M.Sc., Chemistry (University Department) UNDER CBCS (With effect from 2018-19) The course of study and scheme of examinations

Subject	Paper Code	General Title	Ins. Hrs./ Week	Cre -dit	Exam hrs	Max. Marks		
						IA	UE	Total
		1st Year: I Semester						
Core-1	MDCH11	Organic Chemistry – I	5	4	3	25	75	100
Core-2	MDCH12	Inorganic Chemistry – I	5	4	3	25	75	100
Core-3	MDCH13	Physical Chemistry – I	5	4	3	25	75	100
Elective -1	MDCH14A	A. Medicinal and Heterocyclic Chemistry **OR**	3	3	3	25	75	100
	MDCH14B	B. Chemistry of Macromolecules **OR**						
	MDCH14C	C. Organic Analytical Techniques						
Practical-1	MDCH15	Organic Chemistry Practical - I	4	3	6	25	75	100
Practical-2	MDCH16	Inorganic Chemistry Practical - I	4	3	6	25	75	100
Practical-3	MDCH17	Physical Chemistry Practical - I	4	3	6	25	75	100
		1st Year: II Semester						
Core-4	MDCH21	Organic Chemistry – II	4	4	3	25	75	100
Core-5	MDCH22	Inorganic Chemistry - II	4	4	3	25	75	100
Core-6	MDCH23	Physical Chemistry – II	4	4	3	25	75	100
Compul -sory	MDCHR20	Human Rights	2	2	3	25	75	100
Elective -2	MDCH24A	A. Supramolecular and Nano Chemistry **OR**	4	3	3	25	75	100
	MDCH24B	B. Inorganic Photochemistry **OR**						
	MDCH24C	C. Materials Chemistry						
Practical-4	MDCH25	Organic Chemistry Practical – II	4	3	6	25	75	100
Practical-5	MDCH26	Inorganic Chemistry Practical -II	4	3	6	25	75	100
Practical-6	MDCH27	Physical Chemistry Practical - II	4	3	6	25	75	100

***IA = Internal Assessment**
***UE = University Examination**

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Subject	Paper Code	General Title	Ins. Hrs./ Week	Cre -dit	Exam hrs	Max. Marks		
						IA	UE	Total
2nd Year: III Semester								
Core-7	MDCH31	Organic Chemistry – III	4	4	3	25	75	100
Core-8	MDCH32	Inorganic Chemistry – III	4	4	3	25	75	100
Core-9	MDCH33	Physical Chemistry – III	4	4	3	25	75	100
Elective -3	MDCH34A	A. Green and Industrial Chemistry **OR**	3	3	3	25	75	100
	MDCH34B	B. Surface Analytical Techniques and Chemical, Electrochemical and Biosensors **OR**						
	MDCH34C	C. Computational Methods in Chemistry and Chemometrics						
Practical-7	MDCH35	Organic Chemistry Practical – III	5	3	6	25	75	100
Practical-8	MDCH36	Inorganic Chemistry Practical - III	5	3	6	25	75	100
Practical-9	MDCH37	Physical Chemistry Practical – III	5	3	6	25	75	100
2nd Year: IV Semester								
Core-10	MDCH41	Organic Chemistry-IV	4	4	3	25	75	100
Core-11	MDCH42	Scientific Research Methodology	4	4	3	25	75	100
Elective-4	MDCH43A	A. Applications of Spectral Techniques to Inorganic Compounds **OR**	4	3	3	25	75	100
	MDCH43B	B. Instrumental Methods of Analysis **OR**						
	MDCH43C	C. Environmental Chemistry						
Core-12	MDCH44	Project	18	5	-	25	75	100
		Total	**120**	**90**				**2600**

Core (11 Theory Papers + 9 Practicals)	: 69	Credits - 2000 marks
Elective (4 Theory Papers)	: 12	Credits - 400 marks
Compulsory Paper (Human Rights)	: 02	Credits - 100 marks
Project	: 5 Credits	- 100 marks
Total	**: 90 Credits**	**- 2600 Marks**

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FIRST YEAR
SEMESTER-I

CORE–1 **ORGANIC CHEMISTRY-I**
(Stereochemistry and Reactive Intermediates)

Paper Code: MDCH11
Total hours : 75

Course Objectives:

- On successful completion of the course, the students should have a versatile knowledge of aromaticity and to understood the principles and reaction mechanism involving various reactive intermediates.
- The course also aims to explain basic concepts in stereo chemistry and conformational analysis of organic molecules.

Course Out comes: After studying this course the students will be able to:

CO 1. The Student should be learning the Aromaticity of aromatic, Antiaromatic and Non- aromatic systems. Then also learn benzenoid and Non benzenoid system.
CO 2. On effective conclusion of the way, the students should have a useful awareness of Stereochemistry, conformational analysisand three dimensional views of the compound it well use full for the unit.
CO 3. Proceeding actual assumption of the way, the students should have a useful awareness of conformational analysis and three dimensional views of the compound it well use full for the unit.
CO 4. On this paper effective end of the progress, the students should must a flexible understanding of reactive intermediates and their study of cationic, anionic, and free radical formation reaction also study in this unit.
CO 5. On prosperous close of the sequence, the students should have a handy acquaintance of Electrophilic, nucleophilic addition reaction and some important naming reaction also study in this unit.

UNIT-I AROMATICITY

Generalization of Aromaticity: Hückel's 4n + 2 Rule, Craig's rule, Aromatic, Anti-aromatic and Non-aromatic Systems. Aromaticity of benzenoid and non-benzenoid compounds, Annulenes;Fulvenes and Related Systems. Ions-Cations, Anions-Cross-conjugated Polycyclic Systems: Cyclopropenyl Aromatic Systems-Pentalenes, Heptalenes, Azulenes - Cyclobutadiene and cyclooctatetraene.

UNIT–II STEREOCHEMISTRY

Newman, Sawhorse and Fisher projection formulae and interconversions; Molecular symmetry and chirality, Classification of Chiral molecules –R-S notation of simple chiral molecules including substituted biphenyls, allenes andspiranes.Re and Si, Pro R and Pro S notations.Illustrations of homotopic, enantiotopic and diastereotopic hydrogen and prochiral carbons with suitable examples. Compounds with two asymmetric carbons - illustrations of *erythro and threo* nomenclature, E-Z notations.

Definition with example: Racemic mixture, Scalamic mixture, Optical purity - Enantiomeric excess. Asymmetric synthesis – Cram's rule.

UNIT-III CONFORMATIONAL ANALYSIS

Conformation of simple 1,2-disubstituted ethane derivatives, disubstitutedcyclohexanes and halocyclohexane and their stereochemical features, conformations and reactivity of cyclohexanol (acylation and oxidation), reduction of cyclohexanone, esterification and hydrolysis of cyclohexane carboxylic acid derivatives. Sterochemistry of cis and trans decalines, hydrindanes and cyclohexene.

UNIT-IV REACTIVE INTERMEDIATES

Carbocations, carbanions, free radicals, radical cations, radical anions, carbenes and nitrenes, arynes – generation, stability: factors affecting stability (carbocation and carbanion), structure and their reactions in C-C bond and other multiple bond formation.

UNIT-V ADDITION REACTIONS

Electrophilic and nucleophilic addition reaction to C=C: Syn and anti additions, Electrophilic addition reactions via halonium & carbocation intermediate, hydroboration, regio- & stereochemistry, electrophilic addition to conjugated dienes, Nucleophilic addition to C=X (X = O, NR): Hydroboration, Michael addition, Mannich, Stobbe, Darzen, Wittig, Wittig - Horner and Benzoin reactions. Stereochemical aspects to be studied wherever applicable

Reference books

1. Advanced Organic Chemistry part-A. F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)
2. Ernest L. Eliel, Stereochemistry of carbon compounds, T.M.H. Edn., Tata McGraw-Hill Publishing Company, 1962.
3. P.S.Kalsi, Stereochemistry – Conformation and Mechanism, New Age International (P) Ltd. 7th Ed., 2008.
4. D.Nasipuri, Stereochemistry of Organic Compounds, New Age International Publishers, 1994.
5. Ernest L. Eliel, Samuel H. Wilen, Sterochemistry of organic compounds, John Wiley & Sons, 2008.
6. Michael B. Smith, Jerry March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, John Wiley & Sons, 2007.
7. P.S. Kalsi, Stereochemistry and Mechanism through solved problems, Second Edition, New Age International Publishers, 1994.
8. I. L. Finar, Organic Chemistry, 5thEdn., Vol.2, Stereochemistry and Chemistry of Natural Products, Pearson, 2014.
   T.L. Gilchrist and C.W. Rees, Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London.

CORE-2 **INORGANIC CHEMISTRY-I**

(Main Group and Coordination Chemistry)

Paper Code: MDCH12

Course Objectives:

On completion of this course student will have knowledge of

- *Bonding, structure and reactivities of compounds formed by main group elements, and basic knowledge on acid and base concept.*
- *Fundamental theories describe bonding in coordination complexes and structure, stability and reactivity of coordination complexes.*

Course Out comes: After studying this course the students will be able to:

CO 1. To learn the selected crystal structures and to explain what kind of parameters that affects

CO 2. Understand the basic theories of crystal structure of a compound.

CO 3. Basic knowledge on acid and base concept.

CO 4. Fundamental theories describe bonding in coordination complexes.

CO 5. Understand the structure,stability and reactivity of coordination compounds.

UNIT-I MAIN GROUP CHEMISTRY-1

VSEPR- dπ-pπ bonding, Bent's rule; Theories of acid and base. The HSAB concept. Theoretical basis of hardness and softness. Structure and bonding of boranes-diborane and higher boranes, borazines, S-N compounds, phosphazenes and cyclic phosphazene, silicates and silicones; Interhalogen and Noble gas compounds-Hybridisation, Geometry and properties.

UNIT-II THEORIES OF COORDINATION CHEMISTRY

Metal-ligand bonding in transition metal complexes- VBT – CFT and CFSE calculation- MOT for octahedral, square planar and tetrahedral complexes. Factors affecting the magnitude of 10 Dq - evidence for crystal field stabilisation-limitations of VBT, CFT - spectrochemical and Nephelauxetic series, site selection in spinels-Jahn-Teller distortion- MOT for sigma and pi bonding in octahedral complexes and-experimental evidence for pi bonding in octahedral complexes.

UNIT-III STRUCTURE OF COORDINATION COMPLEXES

Structures of coordination compounds - complexes with coordination number one, two, three, four, five and six. - Site preference in trigonal bipyramidal complexes - site preference in square planar complexes - isomerism in five coordinate complexes - Distortion from perfect octahedral symmetry - trigonal prism - geometrical isomerism in octahedral complexes

- optical isomerism in octahedral complexes –Cotton effect- absolute configuration of complexes - stereoselectivity and conformation of chelate rings.

UNIT-IV SUBSTITUTION REACTIONS

Substitution reactions in square planar complexes – Trans effect- Theories of trans effect – the factors affected by square planar complexes - Reaction mechanism and kinetics of nucleophilic substitution in octahedral complexes – the factors affected by octahedral complexes- acid bases hydrolysis – conjugate base mechanism - reaction rates influenced by acid and bases.

UNIT-V STABILITY OF COMPLEXES AND ELECTRON TRANSFER REACTIONS

Labile and inert complexes- stepwise and overall stability of complexes – factors affecting stability of complexes-methods of determination of stability constant (Job's and potentiometric methods)

Mechanisms of electron transfer reactions - outer sphere mechanisms - excited state outer sphere electron transfer reactions - inner sphere mechanisms – atom transfer reaction-Marcus-Hush theory- mixed valent complexes-

Reference Books

1. Inorganic Chemistry - Principles of structure and reactivity, Fourth Edition, J. E. Huheey, E. A. Keiter and R. L. Keiter - Addition Wesley Publishing Co, NY, 1993.
2. Advanced Inorganic Chemistry - F. A. Cotton and G. Wilkinson
3. Mechanism of Inorganic reactions - F. Basolo and R. G. Pearson
4. Inorganic Chemistry - R. B. Heslop and P. L. Robinson
5. Introduction to Ligand Fields - B. N. Figgis - Wiley Eastern Ltd, New Delhi, 1976.
6. Inorganic Chemistry- Gary L.Miessler and Donald A. Tarr, person education, Inc
7. Inorganic electronic spectroscopy, A.B.P.Lever, Elsevier.
8. Coordination Chemistry by S F A Kettle, EIBS, 1973.
9. K. F. Purcell and J. C. Kotz, Inorganic Chemistry,-WB Saunders Co., USA, 1977.
10. W. E. Additson, Structural Principle in Inorganic Chemistry, Longman, 1961.
11. A. F. Wells, Structural Inorganic Chemistry, Oxford, V Edition, 1984.
12. Gary Wulfsberz, Inorganic Chemistry.

CORE-3

PHYSICAL CHEMISTRY-I

(Thermodynamics and Chemical Kinetics)

Paper Code: MDCH13

Course Objectives:

- To know the limitations of classical thermodynamics in the evaluation of macroscopic properties.
- To understand the principles of activity and fugacity.
- To know the theories of kinetic activity.
- To study the techniques of fast reactions.
- To learn about the various surface phenomena.

Course Out comes: After studying this course the students will be able to:

CO1. The limitations of classical thermodynamics in the evaluation of macroscopic properties.

CO2. The various principles involved in group theory

CO3. The theories of catalytic activity

CO4. The principles and selection rules for IR and Raman spectroscopy.

CO5. The symmetry of hybrid orbitals.

UNIT-I THERMODYNAMICS AND NON-IDEAL SYSTEMS

Concepts of Partial Molar Properties-Partial Molar Free Energy and Partial Molar Volume. Chemical potential-Variation of chemical potential with temperature and pressure, Van't Hoff isotherm.

Fugacity–Determination of fugacity of gases by graphical method-Variation of fugacity with temperature and pressure -Lewis Randal rule-Duhem-Margules equation. Determination of activity and activity coefficient of non-electrolyte (EMF method)-Excess functions.

UNIT-II IRREVERSIBLE THERMODYNAMICS

Nernst heat theorem-Third law of thermodynamics-Applications of third law-Entropy change-Calculation of absolute entropies-Apparent exceptions to third law- Non-equilibrium thermodynamics-Basic concepts-Forces and fluxes-Entropy of irreversible processes-Entropy production-Clausius inequality-Phenomenological equations-Onsager reciprocity relations-Coupled reactions.

UNIT-III CHEMICAL KINETICS-I

Potential energy surfaces and Contour diagrams-Microscopic reversibility - Steady–state approximation- Theory of Absolute Reaction Rates- Probability factor-Comparison of transition state theory with collision theory-Eyring equation-Significance of entropy and enthalpy of activation-Linear free energy relationships (LFER) -Hammett and Taft equations-Kinetic isotopic effect.

UNIT-IV CHEMICAL KINETICS-II

Application of ARRT to reaction in solutions - Influence of ionic strength (Bjerrum-Bronsted equation) and dielectric constant on rates in solution-Acid-Base catalysis-Mechanism-Bronsted catalysis law. Kinetics of consecutive reactions.

Enzyme Catalysis-Michaelis-Menten equation-Effect of pH and temperature on enzyme catalyzed reactions-Inhibition of enzyme catalyzed reactions
Fast reactions-Laser Flash photolysis, flow technique and relaxation methods.

UNIT-V SURFACE CHEMISTRY AND CATALYSIS

Chemisorption and Physisorption; Langmuir's adsorption isotherm; - Mechanisms of reactions on surfaces (Rideal–Eley and Langmuir-Hinshelwood mechanisms); BET isotherm-BET equation-Estimation of surface area.
Surface active agents-Classification of surface active agents, Micelles and Reverse Micelles-Critical Micellar Concentration (CMC), Factor affecting the CMC of surfactants.

Reference Books

1. S. Glasstone, Thermodynamics for Chemists, East West Press Pvt. Ltd., New Delhi, 2009.
2. J. Rajaram and J.C. Kuriacose, Thermodynamics for students of chemistry, Pearson, Chennai, 2013.
3. I.M. Koltz and R.M. Rosenberg, Chemical thermodynamics, Benjamin publishers, California, 1972.
4. R. Hasee, Thermodynamics of Irreversible Process, Addition Wesley, Reading.
5. Thomas Engel and Philip Reid, Physical Chemistry, Third Edition, Pearson, 2014.
6. P.W. Atkins, Physical Chemistry,7thedn, Oxford University press, 2002.
7. K.J. Laidler, Chemical Kinetics, Pearson, 5th edition, 2011.
8. J. Rajaram and J.C. Kuriacose, Kinetics and Mechanisms of chemical transformations: Application to Femtochemistry, McMillan, 2011.
9. Agarwal, Basic chemical kinetics, Tata McGraw-Hill, 1990.
10. R.G. Frost and Pearson, Kinetics and mechanism, Wiley, New York.

11. A.W. Adamson, Physical chemistry of surfaces, 6th Ed., Wiley, 1997.
12. G.A. Somorjai, Introduction to surface chemistry and catalysis, John Wiley, 1994.
13. Maron and Prutton, Principles of physical chemistry, McMillan.
14. W.J. Moore, Physical Chemistry, Orient Longman, London (1972).

ELECTIVE – 1A MEDICINAL AND HETEROCYCLIC CHEMISTRY

Paper Code: MDCH14A

Course Objectives:

- Students should be able to understand concepts of drug design and mechanism of drug action of different drugs.
- Students will be aware of metabolism and delivery methods of different classes of drugs.

Course Out comes: After studying this course the students will be able to:

CO1: Students should be able to understand concepts of drug discovery, drug metabolism and lead Optimization methods. Students will be aware of metabolism and delivery methods of different classes of drugs.

CO2: On successful completion of the paper Students should be able to understand concepts of drug design, and pro drug concepts.

CO3: This unit study for mechanism of drug action of different drugs. The Students should be able to understand concepts.

CO4: This unit study for Heterocyclic reaction of fiver member and six membered ring system and also study for the synthesis and proper mechanism.

CO5: This unit study for Condensed Heterocyclic reaction of fiver member and six membered ring system and also study for the synthesis and proper mechanism.

UNIT-I DRUG DISCOVERY

An introduction to drugs and receptors, Drug-Receptor interactions, Neurotransmission-Neurotransmitters.
History of drug discovery, Strategies in lead discovery: Ethnopharmaceutical sources, Plant sources, Animal sources, marine sources, drug metabolism studies, observation of side effects.
Lead Optimization methods: Stereochemistry, Bioisosterism, SAR studies.

UNIT-II DRUG DESIGN

Drug design strategies-Rational drug design: Inhibitors of ACE; Structure based drug design: Anti HIV agents; Ligand based approach.
Design of agonist and antagonist: β_2-Agonists and the treatment of asthma, Discovery of the H2–receptor antagonists

Pro drug concept: prodrugs of ampicillin, elanapril, propranolol.

UNIT-III DRUG ACTION

Pharmacological activity – Antibiotics: Penicillin; Antimalerials: Trimethoprim; NSAIDS: Paracetamol, Ibuprofen, Diclophenac sodium, Antidepressants: Fluoxetine, Anti-histamines, Anti-tuberclosis agents: Isoniazide , Anti-cancer agents: Vinblastine, Taxol

Unit-IV HETEROCYCLICS

Synthesis and reactions of furan, pyrrole, thiophene and pyridines: Furans-Fiest-Benary furan synthesis, Pyrroles and pyrrolidines-Barton. Zard reaction. Hofmann-Loffler-Freytag reaction. Thiophenes-Hinsberg synthesis of thiophene derivatives. Pyridines- Hantzsch (Dihydro)-pyridine synthesis. Skraup/Doebner von Miller reaction.

UNIT-V CONDENSED HETEROCYCLES

Synthesis and reactions of Indole, Quinolines and Isoquinolines: Indoles. Indoles - Fischer indole synthesis, Madelung indole synthesis, Nenitzescu indole synthesis. Quinolines and isoquinolines- Bischler-Napieralski reaction. Friedlander synthesis. Meth-Cohn quinoline synthesis. Pfitzinger quinoline synthesis.

Reference Books

1. Burger's Medicinal Chemistry & Drug discovery, Vol 1-3, 5th Ed, 1995.
2. Chemistry of drug design and drug action-. R. B. Silverman (2004) Acad. press.
3. Graham Patrick, An Introduction to Medicinal Chemistry- 2ndEdn. Qxford, 2010
4. N. K. Jain, Advances in Controlled and Novel Drug Delivery, CBS, 2001.
5. Lednicer, The Organic Chemistry of Drug Synthesis, Vol. 1, 5th Edition, John Wiley & Sons, 2001.
6. Foye's Principles of Medicinal Chemistry, Sixth Edition, Wolters Kluwer, 2008.
7. G.R. Chatwal, Medicinal Chemistry, Himalaya Publishing House.
8. V.K. Ahluwalia and M. Chopra, Medicinal Chemistry, Ane Book Pvt. Ltd., 2008.

ELECTIVE -1B CHEMISTRY OF MACROMOLECULES

Paper Code: MDCH14B

Course Objectives:

- To gain the knowledge in the preparation, properties, characterization and Uses of polymers and bio macromolecules.

Course Out comes: After studying this course the students will be able to:

CO1: To gain the Knowledge of synthesis of macromolecules.

CO2: To understand the structure and properties of macromolecules

CO3: To know the liquid crystal polymers of macromolecules

CO4: To understand the preparation and application of industrial polymers

CO5: To study the structure and role DNA and RNA

UNIT – I INTRODCUTION AND SYNTHESES OF MACROMOLECULES

Introduction, Colloids, Macromolecules, Synthetic Polymers, Biological Polymers, Macromolecular Science.
Techniques of polymerization: emulsion, bulk, solution and suspension. Mechanism of polymerization : free radical, cationic, anionic and co-ordination polymerization (Ziegler - Natta Catalyst), Living Polymers, Coordination Polymerization, Stepwise Polymerization.

UNIT – II STRUCTURE AND PROPERTIES

Structure - property relationship – Mechanical properties, Thermal properties – Glass transition temperature – Factors affecting Glass transition temperature – crystallinity and melting point – related to structure. B) Polymer characterization and analysis Crystalline nature – X-Ray diffraction – Differential Scanning Calorimetry (DSC) – Thermo Gravimetric Analysis – molecular weight determination – Osmometry (membrane), Viscosity, Ultra centrifuge and Gel Permeation Chromatography.

UNIT III LIQUID CRYSTALS POLYMERS

Mesogens, Polymeric Liquid Crystals, Low-Molecular Weight Liquid Crystals,Main-Chain Liquid-Crystalline Polymers, Side-Chain Liquid-Crystalline Polymers, Segmented-Chain Liquid-Crystalline Polymers.

UNIT – IV INDUSTRIAL NATURAL POLYMERS

Important industrial polymers – preparation and application of polyethylene, poly vinyl chloride, poly urethanes, polytetrafluro ethylene (TEFLON), Nafion and ion – exchange resins.
Importance of natural polymers – application and structures of starch, cellulose and chitosin derivatives.

UNIT-V PROTEINS AND NUCLEIC ACIDS

Proteins: Peptides and their synthesis – Merrifield synthesis, Determination of N-terminal/C-terminal residues, Determination of tertiary structure of Protein, Bio-Synthesis of Proteins. Nucleic Acids: Types of Nucleic Acids-DNA & RNA polynucleotide chain. Components-biological functions. Structure and role of (genetic Code) DNA and RNA (Nucleotides only).

Text Books:

1. F. W. Bill Meyer. Text book of polymer science, III Edition, John Wiley and sons, New York.
2. P. J. Flory. Principles of Polymer Chemistry, Cornell Press (recent edition).
3. V. R. Gowarikar, B. Viswanathan, J. Sridhar, Polymer Science – Wiley Eastern, 1986.
4. G. S. Misra – Introduction to Polymer Chemistry, Wiley Eastern Ltd.,
5. P. Bahadur, N. V. Sastry, Principles of Polymer Science, Narosa Publishing House.
6. G. Odian, Principles of Polymerization, McGraw Hill Book Company, New York, 1973.

ELECTIVE – 1C ORGANIC ANALYTICAL TECHNIQUES

Paper Code: MDCH14C

Course Objectives:

- The students should be able to know the purification and extraction techniques.
- This paper enables a student to understand the basic principles of various chromatographic techniques.
- The students should be able to understand the advanced microscopic techniques.

Course Out comes: After studying this course the students will be able to:

CO1: The students should be able to know the purification and extraction techniques

CO2: To Understand the solvent extraction methods of principle and techniques

CO3: The Students gain the knowledge in paper, thin layer and column chromatography methods

CO4: To know the principle and techniques of Zeolites as ion-exchangers and its applicatios

CO5: The students should be able to understand the advanced microscopic techniques

UNIT-I PURIFICATION TECHNIQUES

Desiccants: types and choice of desiccants, drying of solids. Precipitation: types of precipitation, factors affecting the precipitation. Distillation: theory of distillation. Fractional, steam, azeotropic, vaccum distillations.Recrystallization, Sublimation.

UNIT-II EXTRACTION TECHNIQUES

Solvent extraction: Principle and techniques. Distribution ratio and distribution coefficient. Factors affecting extraction efficiency: Role of chelating ligands, crown ethers, calixarenes and cryptands in solvent extraction. Introduction to Solid phase extraction (SPE) and Microwave assisted extraction (MAE). Applications.

UNIT-III CHROMATOGRAPHY

Definition and Classification. Techniques used in Paper, Thin Layer and Column chromatography. Principle, instrumentation and applications of Gas chromatography(GC), Gas-Liquid chromatography (GLC), High performance liquid chromatography (HPLC),. Applications in qualitative and quantitative analysis.

UNIT-IV ION EXCHANGE CHROMATOGRAPHY

Principle and technique. types of ion exchangers.ion exchange equilibria.Ion exchange capacity. effect of complexing ions. Zeolites as ion-exchangers. Applications. Paper electrophoresis.

UNIT-V MICROSCOPIC ANALYSES

Scanning Electron Microscopy, Tunneling Electron Microscopy, Scanning Tunneling Microscopy and Atomic Force Microscopy- Principle, Instrumentation and Applications.

Reference books

1. D.A. Skoog, Principles of Instrumental Analysis, Saunders College Pub.Co, III Edn., 1985
2. A.I Vogel, Text Book of Quantitative Organic Analysis, ELBS III Edn, 1987.
3. D.A.Skoog and D.M.West Fundamentals of Analytical Chemistry, Holt Rinehart and Winston Publications, IV Edn, 2004.
4. Willard, Merit, Dean and Settle, Instrumental Methods of Analysis, CBS Publishers and Distributors, IV Edn.,1989
   G. D. Christian and J.E.O Reilly, Instrumental Analysis, Allyn and Bacon Inc, II Edn., 1986.

PRACTICAL-1 ORGANIC CHEMISTRY PRACTICAL – I

Paper Code: MDCH15

Course Objectives:

- To understand identification of components in the mixture.

Course Out comes: After studying this course the students will be able to:

CO 1: To familiarize the systematic producers organic substances analysis

CO2: To learn two stage preparation involving molecular rearrangement oxidation.

CO3: To know the preparation involving nitration and bromination

CO4: To familiarize the test involving identification of special elements

CO5: To learn the confirmatory test for various functional groups.

1. Identification of components in a two component mixture and preparation of their derivatives- Any six binary mixtures.

2. Determination of m.p. of solid compounds/derivatives.

Reference Books

1. Arthur I. Vogel, “A Textbook of Practical Organic Chemistry”, ELBS.
2. N.S. Gnanapragasam and B. Ramamoorthy, “Organic Chemistry Lab Manual” (2006), S. Visvanathan Printers & Publishers.
3. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern Limited.
4. Mann and Saunders, Laboratory manual of Organic Chemistry.

PRACTICAL-2 INORGANIC CHEMISTRY PRACTICAL – I

Paper Code: MDCH16

Course Objectives:

- To understand the analysis of inorganic mixture and find out the four radicals.

Course Out comes: After studying this course the students will be able to:

CO1: To Know the Qualitative analysis of inorganic mixture.

CO2: Analysis of the various inorganic mixture of compounds.

CO3: Understand the procedure to determine the rare earth elements.

CO4: Know the separation techniques of rare earth elements.

CO5: To get knowledge of Separation of inorganic elements.

Semimicro qualitative analysis of inorganic mixture containing two common and two rare earth cations.

The following are the rare earth cations to be identified.

W, Se, Te, Mo, Ce, Th, Ti, Zr, V, Be, U, Li.

PRACTICAL-3 PHYSICAL CHEMISTRY PRACTICAL – I

Paper Code: MDCH17

Course Objectives:

- To understand the acid hydrolysis and iodination of acetone.

Course Out comes: After studying this course the students will be able to:

CO1: Acid Hydrolysis of ester

CO2: Kinetics of iodination of acetone

CO3: Study of Association of Benzoic acid in Benzene

CO4: Study of phase diagram of two components forming simple eutectic.

CO5: Study of the salt effect on the reaction between acetone and iodine**.**

1. Kinetics – Acid Hydrolysis of Ester – Comparison of strengths of acids.
2. Kinetics – Acid Hydrolysis of Ester – Determination of Arrhenius parameters.
3. Kinetics – Persulphate – Iodide Reaction – Determination of order, effect of Ionic strength on rate constant.
4. Kinetics of saponification of ester.
5. Primary salt effect for the reaction between persulphate and iodide.
6. Kinetics of iodination of acetone.
7. Distribution Law – Study of Association of Benzoic Acid in Benzene.
8. Adsorption –Oxalic Acid/Acetic Acid on charcoal using Freundlich isotherm.
7. Study of phase diagram of two components forming simple eutectic.
8. Study of inversion of cane sugar in the presence of acid using polarimeter.
9. Study the salt effect on the reaction between acetone and iodine.
10. Determination of molecular weight by Rast method.
11. Study of the equilibrium constant of the reaction between KI and I_2.
12. Distribution of acetic acid between water and chloroform.
13. Decomposition of diacetone alcohol-dilatometry method.
14. Complex formation by spectrophotometry-Job's method.

Reference Books

1. Practical Physical Chemistry by B. Viswanathan and P.S. Raghavan, Viva publishers.
2. Findlay's practical Physical Chemistry,'Revised and edited by B.P. Levitt, 9th edn.,Longman, London, 1985.
3. J.N. Gurtur and R. Kapoor, "AdvancedExperiemental Chemistry" Vol. I, S. Chand & Co., Ltd., New Delhi.

SEMESTER-II

CORE-4 **ORGANIC CHEMISTRY-II**

(Organic Reaction Mechanisms and Rearrangements)

Paper Code: MDCH21

Course Objectives:

- This paper explains the basic concepts of substitution reaction and elimination reaction. Mechanism of some of the important rearrangements and named reactions in organic chemistry will be discussed.
- In addition the students will gain knowledge on reaction mechanism and synthetic application of oxidation and reduction reactions in organic synthesis.

Course Out comes: After studying this course the students will be able to:

CO1: This unit explicates the plain theories of substitution Oxidation and reduction reactions in organic synthesis. In calculation the students will advantage information on reaction mechanism.

CO2: This paper explains the basic concepts of substitution reaction and Synthesis techniques of the active group. In addition the students will gain knowledge on reaction mechanism.

CO3: This paper explains the basic concepts of Elimination reaction and Synthesis techniques of sum elimination reactions. In addition the students will gain knowledge on reaction mechanism.

CO4: This red-top describes the elementary concepts of molecular rearrangements reaction in organic chemistry will be discussed. In count the students will advance understanding on reaction mechanism.

CO5: This broadside explains the basic concepts of s naming reaction and reagents in organic synthesis. In addition the students will gain knowledge on reaction mechanism and synthetic application.

UNIT-I **OXIDATION AND REDUCTION REACTIONS**

Oxidation: Carbon Oxidation Number -Calculation. Study of the following oxidation reactions: chromium trioxide, Osmium tetraoxide, DDQ, Chloranil-Alkenes to epoxides and dihydroxy compounds; Oxidation of alcohols using PCC, PDC, Jones, Dess-Martin oxidation; Sharplessepoxidation, Oppenauer oxidation, Oxidation using $Pb(OAc)_4$, SeO_2, Ozonolysis.

Reduction: Selectivity in reduction of 4-t-butylcyclohexanone using selecterides. Hydride reductions - reduction with $LiAlH_4$, $NaBH_4$, tritertiarybutyloxyaluminium hydride, sodium Cyanoborohydride, trialkyltin hydride, hydrazines.MPV reduction, Birch reduction, Asymmetric reduction-Itsuno, Corey and Nyori.

UNIT-II SUBSTITUTION REACTIONS

Aliphatic Substitution Reactions: Mechanism of aliphatic substitution reactions -S_N1, S_N2, S_Ni, mechanism– non-classical carbocations-Neighboring group participation. Substitution at carbonyl, vinylic and
bridgehead systems – substitution by ambident nucleophiles- HVZ reaction, Stark-Enamine reaction.
Aromatic Substitutions: Electrophilic substitution-the arenium ion mechanism. Orientation and reactivity (ortho, meta and para directing groups). Typical reactions including Vilsmeyer - Haack, Schiemann reaction-Synthesis of di and trisubstituted benzene (symmetrical tribromo benzene,
2-amino-5-methylphenol, 3-nitro-4-bromobenzoic acid, 3,4-dibromonitrobenzene) starting from benzene. Nucleophilic substitution - methods for the generation of benzyne intermediate and reactions.Chichibabin reaction.

UNIT-III ELIMINATION REACTIONS

E1, E2 and E1CB mechanism - E1, E2 and E1cB spectrum - Orientation of the double bond -Hoffman and Saytzeff rules - Competition between elimination and substitution. Chugaev and Cope eliminations. Typical eliminations reactions - dehydration, dehydrohalogenation and dehalogenation. Stereochemistry of E2 eliminations in cyclohexane systems. Mechanism of pyrolytic eliminations.

UNIT-IV MOLECULAR REARRANGEMENTS

A detailed study with suitable examples of the mechanism of the following rearrangements: Wagner - Meerwein, Demjanov, Dienone - phenol, Favorski,
Baeyer - Villiger, Sommlet Hauser, Pummerer and Von Richter rearrangements.

UNIT-V NAMED REACTIONS AND REAGENTS IN ORGANIC SYNTHESIS

Reagents: Lithium dialkylcuprates, lithium diisopropylamide(LDA), Dicyclohexylcarbodiimide(DCC), Trimethylsilyl iodide. Named Reactions: Mannich reaction, Biginelli Reaction, Perkin reaction, McMurry coupling, Robinson annulation, Bischler–Napieralski reaction, Polonowski reaction, Bucherer reaction, Willegerodt and Willegerodt-Kindler reaction.

Reference Books

1. R.T. Morrison, R.N. Boyd, Bhattacharjee, Organic Chemistry, seventh edition, Pearson, 2014.
2. S.H.Pine, J.B. Hendrickson, D.J.Cram and G.S.Hammond, Organic Chemistry, IV Edn., McGraw-Hill Company 1980.
3. P.S.Kalsi, Organic Reactions and Mechanisms, II Edn. New Age International Publishers, 2000.
4. J.M.Harris and C.C. Wamser, Fundamentals of Organic Reaction Mechanisms, John Wiley & Sons, Inc. 1976.
5. Jonathan Clayden, Nick Greeves, Stuart Warren, Organic Chemistry, second edition, Oxford University press, 2012.
6. E.S. Gould, Mechanism and Structures in Organic Chemistry, Holt, New York (1959).
7. McMurry,OrganicChemistry,V Edition, Asian Books Pvt Ltd (2000).
8. R.O.C. Norman, Organic Synthesis, Chapman and Hall, NY(1980).
9. S.M. Mukherji and S.P. Singh, Organic Reaction Mechanism, MacMillan India Ltd., Chennai (1990).
10. Peter Sykes, A Guide book to mechanism in organic chemistry, Pearson Edn., (2006).

CORE- 5 # INORGANIC CHEMISTRY-II

(Bioinorganic and Organometallic Chemistry)

Paper Code: MDCH22

Course Objectives:

- On completion of the course the students will have the knowledge about basic concepts and functions of Bio-Inorganic complexes.
- Basic concepts of bonding and catalysis in organ metallic chemistry.

Course Out comes: After studying this course the students will be able to:

CO1: Basic concepts and functions of Bio-Inorganic complexes.

CO2: Understand the Mechanism of various biological reaction in Bio inorganic Chemistry

CO3: Know the mechanisms of Organic metallic compounds in Bio inorganic Complexes.

CO4: Basic concepts of bonding and catalysis in organic metallic compounds.

CO5: Understand the Concept of Organic metallic Compounds.

UNIT-I BIO-INORGANIC CHEMISTRY-I

The role of metal ions in basic biological reactions-vanadium, chromium, manganese, cobalt, molybdenum, tungsten and nickel- transport and storage of metals- sodium- potassium pump- hemoglobin and myoglobin-oxygen transport mechanism-structure and function of hemoglobin and myoglobin- fixation of nitrogen-nitrogen cycle

UNIT II BIO-INORGANIC CHEMISTRY II

Metal containing enzymes- carboxy peptidase- A-structure and reactivity-iron sulphur protein: general features-rubredoxin(Rd)- Ferrodoxins(Fd)-cytochrome C oxidase-cytochrome P450- structure and reactivity-vitamin B12-biochemical function.

UNIT–III ORGANOMETALLICS-1

Definition of organometallic compound- Types of Ligands- hapticity- 18 electron rule-limitation to 18 electron rule-synthesis and structure-metal carbonyl-metal nitrosyl-metal alkene(Zeise's salt)-metallocene-ferrrocene - isolobal concept.

UNIT-IV ORGANOMETALLICS-2

Synthesis, structure and reactivity- metal alkyls- M-C bond cleavage reaction-insertion of CO to M-C bonds- study of mechanism- metal allyls, aryls and arene complexes- multidecker complexes-Synthesis, and reactivity.

UNIT-V ORGANOMETALLIC COMPOUNDS IN CATALYSIS

Organometallic compounds in catalytic reactions – classification- oxidative addition- reductive elimination- insertion- migration- nucleophilic substitution- reactions of coordinated ligands - isomerisation of alkenes-hydrogenation(Wilkinson's catalyst) – hydroformylation (oxo process)-oxidation of olefins(Wacker process) - hydrosilation of alkenes -alkene polymerisation and oligomerisation- Zeigler-Nata catalyst - fluxional molecules.

Reference Books

1. Organometallics 1, complexes with transition metal-carbon -bonds, Bockmann, Oxford science publications, Oxford, 1996.
2. Organometallics 2, complexes with transition metal-carbon -bonds, Bockmann, Oxford science publications, Oxford, 1996.
3. Basic organometallic chemistry, J. Haiduc and J. J. Zuckerman, Walter de Gruyter, Brelin, 1985.
4. Inorganic Chemistry - Priciples of structure and reactivity, J. E. Huheey Harper International Edition, Harper and Rone New York, 1978.
5. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, Fourth Edition.
6. Inorganic Chemistry- Gary L. Miessler and Donald A. Tarr, pearson education, Inc
7. B. Cornils and W.A> Herrmann, Applied homogeneous catalysis, Wiley VCH, Weinheim, 2002.
8. R.B. Jordan, Reaction mechanism of Inorganic and organometllic system, Oxford University press, oxford, 1991.
9. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Panima Publishing Company, New Delhi, 1997.
10. W. Kaim and B. Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life , John Wiley & Sons, New York, USA.

CORE-6 # PHYSICAL CHEMISTRY-II

(GROUP THEORY, SPECTROSCOPY and QUANTUM CHEMISTRY)

Paper Code: MDCH23

Course Objectives:

- Learn about the various principles and applications involved in group theory.
- To know the knowledge about the construction of character tables.
- To understand the principles and selection rules for IR and Raman spectroscopy and symmetry of hybrid orbital's.
- To become familiar with the required mathematics for operators and their applications in quantum mechanical problems.
- To become familiar with the required mathematics for solving quantum mechanical problems.
- To learn the applications of spectroscopy for the study and structural elucidation of molecules.
- To apply the principles of UV-Visible, IR, and Raman spectroscopy.

Course Out comes: After studying this course the students will be able to:

CO1: The use of chemical kinetics in understanding reaction mechanisms and to apply the theories and concepts of it for homogenous and heterogeneous catalysed reactions.

CO2: The quantum mechanical approach to the atomic and molecular electronic structure.

CO3: The required mathematics for solving quantum mechanical problems.

CO4: The limitations of quantum chemistry and classical thermodynamics in the evaluation of macroscopic properties.

CO5: The concepts of statistical thermodynamics for the study of equilibrium reactions and reaction rates.

UNIT-I GROUP THEORY

Definition of groups, subgroups, Abelian and non-Abelian groups- Multiplication tables-Representation of cyclic groups-Similarity transformation-Symmetry elements and symmetry operations, matrix representation-point groups, Schöenflies notations, Matrix representations - reducible and irreducible representations, characters of representations. Direct product representation. Great Orthogonality Theorem (without proof).

UNIT-II GROUP THEORY AND ITS APPLICATIONS

Construction of character tables using GOT for C_{2v}, C_{3v} and D_{2h}. Selection rules for IR and Raman spectra-Procedure for determining symmetry of normal modes of vibration - Hybrid orbitals in BF_3, CH_4 and NH_3.

Application of group theory for the electronic spectra of ethylene and formaldehyde.

UNIT-III PHASE RULE AND SPECTROSCOPY-I

Phase Rule: Derivation of Gibb's phase rule. Application to three components system-Graphical representation-Systems of three liquids (Chloroform/acetic acid/water; water/silvernitrate/ammonium nitrate).

Classification of molecules (linear, symmetric top and asymmetric top molecules)-Rigid rotor model-Effect of isotopic substitution-Non-rigid rotor-Applications-Vibrational energy expression-zero point energy-force constant and bond strengths-anharmonicity; vibration-rotational spectroscopy-P,Q,R branches-overtones-hot bands-Fermi-resonance; far-IR region.

UNIT-IV SPECTROSCOPY-II

Classical and quantum theories of Raman effect-Stokes' and anti-Stokes' lines-Raman selection rules. Rotational Raman spectra-Vibrational Raman spectra-symmetry and Raman active vibrations, rule of mutual exclusion; Rotation-Vibration Raman spectra of diatomic molecules. Resonance Raman spectroscopy-Coherent anti-Stokes Raman Spectroscopy (CARS)-Applications.

UNIT-V QUANTUM CHEMISTRY-I

Wave-particle dualism, Uncertainty principle. Black body radiation, Planck's radiation law-Photoelectric effect-Compton effect.Spherical polar co-ordinates-Postulates of quantum mechanics. Diagrams of radial and angular wave functions. Radial and angular distribution function and their significance. Operators: Algebra operator, Commutation operator, Linear and Hermitian operator, Hamiltonian operator-Angular momentum operator -eigen functions and eigen values- Physical significance of wave function. Schrödinger equation-Applications of Schrödinger equation to simple systems–Particle in a box-one and three-dimensional box problem-Orthogonalisation and normalisation-QM tunneling.

Reference Books

1. F.A. Cotton, Chemical application of Group theory, 3rd Edition John-Wiley & Sons, Singapore, 2003.
2. K.V. Raman, Group theory and its applications to chemistry, Tata McGraw-Hill, 1994.
3. V. Ramakrishnan and M.S. Gopinathan, Group theory in chemistry, Vishal publications, 1998.
4. Bhattacharya, Group theory and its applications, Himalaya Publishing House, 1992.
5. R. Chang – Basic principles of spectroscopy, McGraw Hill, New Delhi.
6. C.N. Banwell and E.N. McCash – Fundamentals of Molecular spectroscopy, 5th Edition, Tata McGraw Hill, New Delhi, 2006.
7. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New

York, 2007.
8. Gordon M.Barrow-Physical Chemistry, McGraw Hill Publishing Company Ltd., 2007.
9. R.K. Prasad, Quantum chemistry, Wiley Eastern, 1993.
10. W. Levine, Quantum chemistry, Prentice-Hall, 2000.
11. D.A. McQuarrie, Quantum chemistry, University science books, MilValley, California, 1998.
12. P.W. Atkins, Molecular Quantum mechanics, Clarendon Press New York, 2009.
13. R. Anantharaman, Fundamentals of Quantum chemistry, McMillan India.
14. Thomas Engel and Philip Reid, Quantum Chemistry and Spectroscopy , Pearson, 6th edition, 2012.
15. A. K. Chandra, Introductory quantum chemistry, 4th ed,. Tata McGraw Hill 1994.
16. H.K. Moudgil, Text Book of Physical Chemistry, PHI Learning, New Delhi, 2010.

SUPRAMOLECULAR AND NANO CHEMISTRY
ELECTIVE-2A

Paper Code: MDCH24A

Course Objectives:

- On completion of the course the student should know the basis of suprmolecular chemistry, metal-organic framework solids, nano mateirlas and their applications.
- Various techniques available to characterize the advanced Inorganic materials

Course Out comes: After studying this course the students will be able to:

CO1: To know the basis of supramolecular Chemistry, meat-organic framework solids,nanomaterials and their applications.

CO2: Various techniques available to characterize the advanced inorganic materials.

CO3: To know the basic concepts of nano chemistry of materials.

CO4: Understand the various techniques of preparation of nano materials.

CO5: Explore the theoretical understanding of various physical and chemical properties of nanomaterials.

UNIT-I SUPRAMOLECULAR CHEMISTRY

Introduction to supramolecular chemistry- Definitions and classification of non-covalent interactions- supramolecular synthons-Molecular recognition-self assembly-Supramolecular chemistry of metal containing compounds-1D, 2D, 3D- Host-Guest compounds-Alpha-, Beta-, Gamma-cyclodextrins..

UNIT-II FRAMEWORK SOLIDS

Introduction-definition of porosity, pore size, pore volume, pore density-zeolites-synthesis and applications-metal organic frame work solids-definition-classifications-uses of different types of organic ligands- tuning of structure and properties - synthetic methods- Advantage of MOF solids over zeolites-cracking of petroleum products

UNIT-III NANOCHEMISTRY

General introduction to nanomaterials and emergence of nanotechnology; Synthesis of nanoparticles of ZnO_2, TiO_2, silver, gold, rhodium, palladium, platinum, and; carbon materials- fullerene- porous nano carbon(PNC)-synthesis

Techniques of synthesis: electroplating and electro-phoretic deposition, conversion through chemicalreactions and lithography; Thin films:Chemical vapor deposition and Atomic layer deposition techniques; Carbon fullerenes and nanotubes.

UNIT-IV ANALYTICAL TECHNIQUES

Electronic microscopes- SEM – TEM - X-ray diffraction-EXAFS - Nitrogen adsorption-desrption method-TG/DTA/DSC methods-instrumentation and interpretations and applications.

UNIT-V ADVANCED INORGANIC MATERIALS

Applications of Advanced Inorganic materials in catalysis-gas adsorption-gas storage-sensors.

Reference Books

1. Supramolecular chemistry, J.M.Lehn, VCH
2. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, 2, Wiley – VCH, Weinheim, 2004
3. Nanochemistry, Kenneth J. Klabunde and G.B.Sergeev
4. G.Zhong Cao. Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Imperial College Press (2004)
5. *Metal-Organic Frameworks Applications from Catalysis to Gas Storage*. Cejka, J, ed. (2011). Wiley-VCH. ISBN 978-3-527-32870-3
6. *Zeolites and Catalysis: Synthesis, Reactions and Applications*. Jiri Cejka; Avelino Corma; Stacey Zones (2010). John Wiley & Sons. ISBN 978-3-527-63030-1.

ELECTIVE-2B # INORGANIC PHOTOCHEMISTRY

Paper Code: MDCH24B

Course Objectives:

- On the completion of the course the student will have the knowledge of basic principle of inorganic photochemistry
- Instrumentation techniques used in Inorganic photochemistry.
- Application of photochemical properties such as sensitizer of Inorganic compounds.

Course Out comes: After studying this course the students will be able to:

CO1: The students will have the knowledge of basic principle of inorganic photochemistry

CO2: To understand the concept of excited states of metal complexes

CO3: To know the instrumentation techniques used in inorganic photochemistry

CO4: To study the energy transfer under conditions of weak and strong interaction in redox reaction.

CO5: To know the application of photochemical properties such as sensitizer of inorganic compounds

UNIT-I PHOTOPHYSICAL PROCESSES

Absorption, excitation,photochemical laws, quantum yield, electronically excited states, life times-measurements of the times. Flash photolysis, energy dissipation by radiative and non-radiative processes, absorption spectra, Frank-Condon principle, photochemical stages-primary and secondary processes.

UNIT-II METAL COMPLEXES

Excited states of metal complexes: Comparison with organic compounds, electronically excited states of metal complexes, charge transfer spectra, charge transfer excitations.

UNIT-III PHOTOREACTIONS

Photosubstitution, photooxidation and photoreduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy

content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.

UNIT-IV REDOX REACTIONS

Energy transfer under conditions of weak interaction and strong interaction-examples formation; condition of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates, (2,2-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidising character of $[Ru(bipy)_3]^{2+}$ complex, comparison with $[Fe(bipy)_3]^{2+}$;role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light.

UNIT-V APPLICATIONS

Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction.

Reference Books:

1. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley.
2. Inorganic Photochemistry, J.Chem. Educ. vol. 60 No. 10, 1983.
3. Progress in Inorganic Chemistry, Vol. 30ed. S.J. Lippard. Wiley. Coordination Chem. Revs. 1981, vol. 39, 121, 1231, 1975, 14, 321,; 1990 97, 313.
4. Photochemistry of Coordination Compounds, V. Balzari and V. Carassiti, Academic Press. Elements of Inorganic Photochemistry, G.J. Ferraudi, Wiley.
5. S.Arunachalam, "Inorganic Photochemistry - An Introduction to Photochemical andPhotophysical Aspects of Metal Complexes", Kala Publications, Tiruchirappalli, India, 2002.
6. D.M. Roundhill, “Photochemistry and photophysics of Metal complexes”, Springer;Edition, 1994.

ELECTIVE-2C

MATERIALS CHEMISTRY

Paper Code: MDCH24C

Course Objectives:

- On completion of this course the students will have the knowledge of Principle involves in preparative technique, mainly, used to synthesize useful materials Importance of some useful properties of solid materials.

Course Out comes: After studying this course the students will be able to:

CO1: To Understand the role of materials and their classification

CO2: To know the preparative techniques of ceramic materials

CO3: The students gain the knowledge in superconductor materials

CO4: To study the functional organic materials of Fullerenes,ferroelectrics and organic superconductors

CO5: To know the importance of some useful properties of solid materials

UNIT-I MATERIAL DESIGN

Materials and their classification, Role of Chemistry in Material design. General methods of synthesis of inorganic materials–homogeneous nucleation and heterogeneous nucleation, growth of nuclei and factors of importance; synthesis of metallic, semiconductor and metal oxide nano particles.

UNIT-II PREPARATIVE TECHNIQUES

Ceramic methods; chemical strategies, chemical vapour deposition-MOCVD; preparation of nanomaterials, Langmuir- Blodgett Films. Fabrication of ordered nanostructures . Composition and purity of materials.

UNIT-III SUPERCONDUCTORS

Structural features of cuprate superconductors. 1-2-3 and 2-1-4 cuprates; structure. Normal state properties: anisotropy and temperature dependence of electrical resistance. Superconducting state: heat capacity, coherence length, relation between Tc and hole concentration in cuprates; mechanism of superconductivity in cuprates. Applications of high Tc-cuprates.

UNIT-IV FUNCTIONAL ORGANIC MATERIALS

Conducting organics - charge transfer materials and conducting polymers. Organic superconductors. Fullerenes. Molecular ferromagnets and ferroelectrics. Liquid crystals: mesomorphic behaviour, optical properties of liquid crystals, display devices.

UNIT-V NLO MATERIALS

Second and third order non-linear effects; molecular rectifiers and frequency doublers; unimolecular electronic devices. Photochromic materials; optical data storage, memory and switches.

Reference Books:

1. A.R. West, Solid State Chemistry and its Applications, (1984) John Wiley & Sons, Singapore.
2. C.N R. Rao and J. Gopalkrishnan, New Directions in Solid State Chemistry, (1997) Cambridge Univ. Press.
3. T. V. Ramakrishnan and C.N.R. Rao, Superconductivity Today, (1992) Wiley Eastern Ltd., New Delhi.
4. P. Ball, Designing the Molecular World: Chemistry at the Frontier, (1994) Princeton Univ. Press.

COMPULSORY PAPER **HUMAN RIGHTS**

Paper Code: MDHR20

Course Objectives:

- To understand historical development and theories- international human rights.

Course Out comes: After studying this course the students will be able to:

CO1: Apply effective written and oral communication skills to business and legal situations.

CO2: Analyze the global legal environment

CO3: Students will graduate with the ability to analyze complex problems, find and deploy a variety of legal authorities, and communicate effectively in a variety of Settings

CO4: Use critical thinking skills in business situations.

CO5: Apply an ethical understanding and perspective to business situations.

UNIT-I HISTORICAL DEVELOPMENT AND THEORIES

Definition of Human Rights - Nature, Content, Legitimacy and Priority - Theories on Human Rights - Historical Development of Human Rights.

UNIT-II INTERNATIONAL HUMAN RIGHTS-1

Prescription and Enforcement up to World War II - Human Rights and the UNO- Universal Declaration of Human Rights - International Covenant on Civil and Political Rights - International Covenant on Economic, Social and Cultural Rights and Optional Protocol.

UNIT-III HUMAN RIGHTS DECLARATIONS

U.N. Human Rights Declarations - U.N. Human Commissioner.

UNIT-IV INTERNATIONAL HUMAN RIGHTS-2

Amnesty International - Human Rights and Helsinki Process – Regional Developments - European Human Rights System - African Human Rights System - International Human Rights in Domestic courts.

UNIT-V HUMAN RIGHTS FOR CHILDREN AND WOMEN

Contemporary Issues on Human Rights: Children's Rights - Women's Rights - Dalit's Rights - Bonded Labour and Wages - Refugees - Capital Punishment. Fundamental Rights in the Indian Constitution - Directive Principles of State Policy - Fundamental Duties - National Human Rights Commission.

Reference Books

1. International Bill of Human Rights, Amnesty International Publication, 1988.

2. Human Rights, Questions and Answers, UNESCO, 1982
3. Mausice Cranston - What is Human Rights
4. Desai, A.R. - Violation of Democratic Rights in India

6. Timm. R.W. - Working for Justice and Human Rights.
7. Human Rights, A Selected Bibliography, USIS.
8. J.C.Johari - Human Rights and New World Order.

10. Amnesty International, Human Rights in India.
11. P.C.Sinha-International Encyclopedia of Peace, Security
12. K. Cheous (Ed) Social Justice and Human Rights (Vols 1-7).
13. Devasia, V.V. - Human Rights and Victimology.

Magazines:

1. The Lawyer, Bombay
2. Human Rights Today, Columbia University
3. International Instruments of Human Rights, UN Publication
4. Human Rights Quarterly, John Hopkins University, U.S.A.

PRACTICAL-4 **ORGANIC CHEMISTRY PRACTICAL – II**

Paper Code: MDCH25

Course Objectives:

- To understand the purifications techniques.

Course Out comes: After studying this course the students will be able to:

CO 1: Perform the ternary mixtures.

CO2: Preparation of organic compounds, their purifications and run TLC.

CO3: Determination of physical constant: Melting point, Boiling point.

CO4: Different separation techniques.

CO5: Extract, identify and characterize the compounds isolated from natural products.

Any FOUR preparations from the following single stage preparations:

1. Preparation of p-benzoquinone from hydroquinone
2. p-Nitrobenzoic acid from p-nitrotoluene
3. Preparation of 4,6-dimethyl coumarin
4. Benzhydrol from benzophenone
5. Preparation of 2,5-di-t-butylhydroquinone
6. 1,2,3,4 - Tetrahydrocarbazole from cyclohexanone
7. Preparation of dibenzylidene acetone
8. 2,3 - Dimethylindole from phenyl hydrazine and 2 - butanone

Any THREE preparations from the following involving two stages

1. sym-Tribromo benzene from aniline.
2. Benzanilide from benzophenone
3. m-Nitro benzoic acid from methyl benzoate
4. Preparation of 2,4,6-tribromoiodobenzene
5. m-Nitro benzoic acid from benzaldehyde
6. Preparation of p-nitroacetanilde
7. 2-Phenyl indole from phenyl hydrazine
8. 2, 4-dinitrophenyl hydrazine from p-nitrochlorobenzene

Any TWO exercises in the extraction of natural products

Caffeine from tea leaves
Lactose from milk
Citric acid from lemon
Piperine from black pepper

Reference Books

1. Arthur I. Vogel, “A Textbook of Practical Organic Chemistry”, ELBS.
2. N.S. Gnanapragasam and B. Ramamoorthy, “Organic Chemistry Lab Manual” (2006), S. Visvanathan Printers & Publishers.

PRACTICAL-5 INORGANIC CHEMISTRY PRACTICAL – II

Paper Code: MDCH26

Course Objectives:

- To understand the anions and cations estimations techniques.

Course Out comes: After studying this course the students will be able to:

CO 1: Identify various ions present in alloys.

CO2: Prepare and characterize various complexes and analyse the samples throughly.

CO3: Estimate the amount of ions by complexometric and gravimetric methods

CO4: To Know the Basic laws of Photochemistry.

CO5: Understand the concepts of various titrations of Complexometric methods.

Complexometric titrations

Estimation of Ca^{2+}, Mg^{2+}, Zn^{2+} and Ni^{2+} using EDTA

Preparation of the followings:

Potassium tris (33xalate) aluminate (III) trihydrate
Tris (thiourea) copper (I) chloride
Potassium tris (oxalaato) chromate (III) trihydrate
Sodium bis(thiosulphato) cuprate (I)
Sodium hexanitrocobaltate (III)
Chloropentammine cobalt (III) chloride
Bis (acetylacetonato) copper (II)
Hexamminenickel (II) chloride
Bis (thiocyanato) pyridine manganese (II)

Colorimetric Analysis

Photoelectric method: Estimation of iron(III), nickel(III) and manganese(VII).

PRACTICAL-6 PHYSICAL CHEMISTRY PRACTICAL – II

Paper Code: MDCH27

Course Objectives:

- To understand the different techniques**.**

Course Out comes: After studying this course the students will be able to:

CO 1: Determination of the equivalent conductance of a weak acid at different concentrations and verify Ostwald dilution law and calculate the dissociation constant of the acid.

CO2: Determination of equivalent conductance of a strong electrolyte and verification of Debye- Huckel Onsager equation.

CO3: Verification of Ostwald dilution law for a weak electrolyte.

CO4: Determination of Pka values of weak acids and weak bases.

CO5: Conductometric titrations of mixtures of two components. A. Acid – Base titrations. B. precipitation titrations.

Conductometric/Potentiometric Titrations- I

1. Conductometric titrations of mixtures of two components.
   A. Acid-Base titrations.
   B. Precipitation titrations.
   C. Displacement titrations.
2. Conductometric titrations of a mixture of acids (HCl, CH_3COOH) and NaOH.
3. Potentiometric titrations of a mixture of acids.
4. Potentiometric determination of the dissociation constant of weak acid (K_a)

   Using quinhydrone/calomel electrode.
5. Precipitation titrations- $BaCl_2$ vs. $MgSO_4$.
6. Determination of pK_a values of weak acids and weak bases.
7. Determination of solubility product by potentiometry-concentration cell method.

Reference Books

1. B.P. Levitt (Ed.), Findlay's Practical Physical Chemistry**,** 9th edn., Longman, London,1985.
2. J.N. Gurtu and R. Kapoor, Advanced Experimental Chemistry, Vol. I, S. Chand & Co. Ltd., New Delhi, 1980.

SECOND YEAR

SEMESTER-III

CORE-7

ORGANIC CHEMISTRY-III

(Organic spectroscopy and Natural Products)

Paper Code: MDCH31

Course Objectives:

On successful completion of the course the students should have

- Learnt the basic principles of organic spectroscopy
- Learnt the structural analysis using spectral data
- Learnt the syntheses and uses of natural products.

Course Out comes: After studying this course the students will be able to:

CO 1: On successful completion of the course the students should have learnt the basic principles of organic spectroscopy, calculate the number of molecular weight using Woodward - Fisher rules and functional group identification.

CO2: On positive conclusion of the way the students should have well-read the basic principles of organic spectroscopy, calculate the number of proton and carbon present in the compound identification techniques also study in the unit.

CO3: On active completion of the progress the students should have Learn the mass spectrum and fragmentations techniques also study in the unit.

CO4: This unit explicates the plain theories of steroids hormones in organic synthesis. In calculation the students will advantage information on biosynthesis reaction mechanism.

CO5: This paper explicates the plain theories of alkaloids hormones in organic synthesis. In calculation the students will advantage information on biosynthesis reaction mechanism.

UNIT-I UV & IR

UV-Visible spectroscopy: Introduction- Woodward-Fieser rules for conjugated dienes, carbonyl compounds and enones, ultraviolet spectra of aromatic and heterocyclic compounds. IR spectroscopy: Introduction- finger print region – Far IR region Applications of IR spectroscopy to identify alkane, alkene, alkyne, aromatic compounds, nitrile and aromatic residues, Identification of alcohols, ethers, phenols, amines and carbonyl compounds such as ketones, aldehydes, esters, amides, acids, conjugated carbonyls compounds and other functional groups- Effect of hydrogen bonding and effect of solvent on vibrational frequencies.

UNIT-II NMR

Introduction-Nuclear spin states- Nuclear Magnetic moments-Absorption of Energy-Resonance- Instrumentation (Principle only): Continuous wave method, FT NMR-chemical shift and its measurements, factors affecting the chemical shift including anisotropic effect-relaxation processes-Spin-spin coupling-Coupling constant – Multiplicity-Spin systems-NOE effects-1H NMR of simple aliphatic and aromatic compounds. Principles of $_{13}C$ NMR,- proton decoupled and off – resonance $_{13}C$ NMR spectra – DEPT methods- factors affecting 13C chemical shift -$_{13}C$ NMR spectra of

simple organic molecules. Problem solving (for molecules with a maximum number of C10).

UNIT-III MASS & PROBLEM SOLVING

Introduction- Principles- Instrumentation-Ionization techniques such as Chemical ionization, Electron ionization, ESI, FD, FAB, MALDI. Applications of mass spectra to elucidate molecular formula and structure. Mc. Lafferty rearrangement-Nitrogen rule-Interpretation of fragmentation pattern of aliphatic alcohols, aldehydes, esters, ethers, hydrocarbons, carboxylic acids, amines, halogen compounds and simple aromatic compounds. Appearance and significance of isotopic peaks. Structural elucidation of simple organic molecules with the application of spectral techniques-Problems involving combination of spectral data.

UNIT-IV STEROIDS

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry of cholesterol. Isolation, structure determination and synthesis of cholesterol, Biosynthesis of Cholesterol.

Conversion of cholesterol into sex hormones such as androsterone, testosterone, estrone and progesterone.

UNIT V ALKALOIDS

Total Synthesis of Alkaloids: Introduction, Sources of alkaloids, Classification, Preussin, Swainsonine, Horsifiline, Ellipticine and Reserpine (Synthesis only)

Reference Books

1. I.L. Finar, Organic Chemistry, Vol.II, Fifth edn. First Indian reprint, Pearson Education Asia Pvt. Ltd. 2000
2. P.S. Kalsi, Spectroscopy of Organic Compounds, Wiley Eastern Ltd. Madras, 1995.
3. Joseph Lambert, Scott Gronert, Herbert Shurvell, David Lightner, Robert Graham Cooks, Organic Structural Spectroscopy: Pearson New International Edition, 2nd Edition, 2013.
4. William Kemp, NMR in Chemistry, Mac Millan, 1986.
5. Robert M Silverstein, Francis Webster, Kiemle, Bryce. Spectrometric identification of organic compounds, 8th Ed., Wiley. 2014.
6. Jie Jack Li. E. J. Corey, Total Synthesis of Alkaloids, Springer, 2012.

CORE-8 # INORGANIC CHEMISTRY–III

(Solid state and Nuclear Chemistry)

Paper Code: MDCH32

Course Objectives:
After completion of the course the students will have the knowledge of

- Basic concepts describing structure of solids and properties of solids.
- Basis of nuclear chemistry and types of nuclear reactions.

Course Out comes: After studying this course the students will be able to:

CO 1: Know the Basic concepts of Solid State of Matter.

CO2: Know the theroies of Semiconductor, Insulator and super conductors of Solids.

CO3: Understand the Concept of metal clusters in Coordination Compounds.

CO4: Acquire the fundamental knowledge in Nuclear Chemistry.

CO5: Know the Working of Nuclear reaction in Nuclear Chemistry.

UNIT-I BASIC CONCEPTS IN SOLID STATE

Lattice, unit cell, crystal systems and Bravais lattices-Miller indices and labelling of planes –symmetry properties –crystallographic point groups and space groups – fundamentals of X-ray diffraction- Laue equation and Brag's law-powder and single crystal X-ray diffraction-Debye-Scherrer formula-systematic absences, electron and neutron diffraction.

UNIT-II INORGANIC SOLIDS

Ionic bonds- lattice energy of ionic crystals-Born-Haber cycle-Born lande equation-Madelung constant-Structures–cesium chloride-wurtzite–zinc blende –rutile –fluorite. Defects- types of defects-non –stochiometry– point defects in solids –Schottky and Frenkel defects- colour centers – linear defects –dislocations – effects due to dislocations- Metallic state – free electron and band theories- insulator, semiconductor, -intrinsic and extrinsic semi conductors-super conductors.

UNIT-III METAL CLUSTERS

Metal clusters- classification- metal halides and oxides-binuclear clusters-Rhenium dinuclear clusters- structure and bonding-trinuclear clusters, teranuclear clusters and hexanuclear clusters- chevrel phases- Wade's rule-polyatomic zintal anions and cations (naked clusters).

UNIT-IV NUCLEAR CHEMISTRY-1

Nuclear properties: Nuclear spin and moments, origin of nuclear forces, salient features of the liquid drop and the shell models of the nucleus. Models of Radioactive Decay: Orbital electron capture: nuclear isomerism, internal conversion, GM and Scintillation counters. Nuclear Reactions: Types, reactions, cross section, Q-value, nuclear fission and fusion reactions as energy sources; direct reactions; photonuclear and thermo nuclear reactions.

UNIT-V NUCLEAR CHEMISTRY-2

Stellar energy: synthesis of elements, hydrogen burning, carbon burning,
Nuclear Reactors: fast breeder reactors, particle accelerators, linear accelerators, cyclotron and synchrotron.
Radio analytical Methods: Isotope dilution analysis, Radiometric Titrations, Radio immune assay, Neutron activation analysis.

Reference

1. West, A. R. Solid State Chemistry and its Applications, John Wiley & Sons: New York, 1989
2. L.V.Azaroff – Introduction to solids, John Wiley.
3. W.E.Addision – structural principles of Inorganic Chemistry, Longman, 1961.
4. N.B.Hannay – Solid state chemistry, Prentice Hall, New Delhi, 1976.
5. R.A.Alberty and Silby – Solid state chemistry.
6. S.Glasstone – Source book on atomic energy, Von Nostrand Co., 1969.
7. G.Friedlander, J.W.Kennedy, - Nuclear and Radiochemistry, John Wiley and sons, 1981.
8. H.J.Arnikar – Essentials of Nuclear chemistry, Wiley Easter Co., 4thedition, 1995.
9. C. N. R. Rao and J.Gopalakrishnan, New Directions in Solid State Chemistry.

CORE-9 # PHYSICAL CHEMISTRY-III

(Electrochemistry, Quantum and Photochemistry)

Paper Code: MDCH33

Course Objectives:

After this course the student should be able

- To understand the behavior of electrolytes in solution and structure of the electrode surface.
- To differentiate electrode kinetics from other types kinetic studies.
- To know the principle and applications of polarographic techniques.
- To make the students knowledgeable and applications in quantum chemistry.
- To understand and appreciate the quantum mechanical approach to the atomic and molecular electronic structure.
- To learn the applications of photochemistry.
- To learn the principles and applications of statistical thermodynamics and classical thermodynamics in the evaluation of macroscopic properties.
- To understand the inter linking of quantum chemistry and statistical thermodynamics that leads to classical thermodynamics.

Course Out comes: After studying this course the students will be able to:

CO 1: The behaviour of electrolytes in solution.

CO2: The structure of the electrode surface.

CO3: Differentiate electrode kinetics from others types kinetic studies.

CO4: The application of spectroscopy for the study and structural elucidate ion of molecules.

CO5: principles of mass, UV, IR, NMR, ESR, photo electron spectroscopy.

UNIT-I ELECTROCHEMISTRY-I

Elcetrochemistry of solutions: Ionic atmosphere, Kohlrausch law and its applications-Debye-Huckel-Onsagar equation-Derivation-validity and deviation - conductance of high field and high frequency-Electro kinetic phenomena-Electro capillary phenomenon-Lipmann's equation-Zeta potential and its applications. Introduction to electrical double layer-Evidences for electrical double layer. Structure of electrified interface-Helmholtz-Perrin, Guoy-Chapmann and Stern models of electrical double layer.

UNIT–II ELECTROCHEMISTRY-II

Over potential and its significance-Butler-Volmer equation (single step, one electron transfer only) - Exchange current density. Nernst equation as a special case of Butler-Volmer equation–Reaction resistance-Polarisable and non-polarisable

electrodes-Low and high field approximations-Tafel equation.Fuel cells-Classification-Chemistry of fuel cells-detailed description-Ion-selective electrodes.
Polarography: Residual current-limiting current-Ilkovic equation, half wave potential and its significance, polarographic maxima-qualitative and quantitative estimation of metal ions.

UNIT-III QUANTUM CHEMISTRY-II

Applications of wave mechanics- Harmonic oscillator- Rigid rotator-Hydrogen atom solution (No derivation required). Approximation methods–Variation method, Perturbation method for non-degenerate and time-independent system-Slater determinant-Anti-symmetric wavefunctions-Application to Helium atom-Born-Oppenheimer approximation.Spin orbit interaction, L-S and j-j coupling schemes–Hartree-Fock SCF method for many electron systems. Application of HMO treatment to ethylene, butadiene and benzene.

UNIT-IV STATISTICAL THERMODYNAMICS

Objectives of statistical thermodynamics, Concept of distributions, Types of ensembles. Thermodynamic probability, Most probable distribution Law-Classical statistics-Maxwell-Boltzmann (MB) statistics-Quantum statistics-Bose-Einstein (BE) and Fermi-Dirac (FD) statistics-Derivation of distribution function-MB, BE and FD statistics comparison-Partition functions-Translational, rotational, vibrational and electronic partition function (Problem only)- Relation between entropy and partition function; Debye and Einstein heat capacity of solids. Ortho and para hydrogen.

UNIT-V PHOTOCHEMISTRY

Franck-Condon principle-Jablonskii diagram-primary and secondary processes-Flourescence and phosphorescence-Quantum yield-Chemical actionometry-Photosensitization, chemiluminescence.
Kinetics of photochemical processes-H_2 and Cl_2 reaction-Excimers and Exciplexes. Mechanism of fluorescence quenching- Stern-Volmer equation and its applications. Photodegradation of polymers-Atmospheric photochemistry. Photo-voltaic cells-Photo-assisted electrolysis of water-Aspects of solar energy conversion.

Reference Books

1. J.O.M. Bokris and A. K. N. Reddy, Electrochemistry, Vol. 1 and 2, Plenum, New York.
2. S. Glasstone, Introduction to Electrochemistry, Affiliated East West Press,New Delhi.
3. D.R.Crow, Principles and Applications to Electrochemistry, Chapman and Hall (1991).
4. H.Reiger, Electrochemistry, Prentice-Hall International Inc, New York (2012).
5. R.K. Prasad, Quantum chemistry, Wiley Eastern, 1993.
6. W. Levine, Quantum chemistry, Prentice-Hall, 2000.
7. Donald A.McQuarrie, Quantum chemistry, University science books, Oxford University Press,1983 .
8. Thomas Engel and Philip Reid, Thermodynamics: Statistical thermodynamics and Kinetics, Pearson, 2012.
9. M.C. Gupta, Statistical thermodynamics, New Age International, Pvt., Ltd., New Delhi, 1995.
10. F.W. Sears, G.L. SalingarTurcotte; Statistical thermodynamics, Narosa Publishing house New Delhi, 1998.
11. N.J.Turro, Modern Molecular Photochemistry, Benjamin, Cumming, MenloPark, California.
12. K.K.Rohatgi, Mukherjee, Fundamentals of Photochemistry, New Age International Pvt. Ltd, Chennai, 2009.
13. R.P.Wayne, Photochemistry, Butterworths, London.

ELECTIVE-3A GREEN AND INDUSTRIAL CHEMISTRY

Paper Code: MDCH34A

Course Objectives:

After this course the student should be able

- To understand the advantages and importance of green chemistry.
- To look for green chemistry strategies for designing the chemical synthesis.
- To make the students knowledgeable in solar energy conversion.
- To understand the basics of water chemistry.
- To understand the importance of polymers in industries.

Course Out comes: After studying this course the students will be able to:

CO 1: To understand the advantages and importance of green chemistry.

CO2: To look for green chemistry strategies for designing the chemical synthesis.

CO3: To make the students knowledgeable in solar energy conversion.

CO4: To understand the basics of water chemistry.

CO5: To understand the importance of polymers in industries.

UNIT-I GREEN CHEMISTRY

Introduction: Prospects and future of Green Chemistry, Twelve guiding principles of green chemistry. Concept of atom economy. Green starting materials, Green reagents, Green solvents and reaction conditions, Green synthesis- Real world cases (Traditional Vs. Green processes) Synthesis of Ibuprofen, Adipic acid. Biomimetic, multifunctional reagents; Combinatorial green chemistry; Non-covalent derivatization.

UNIT-II MICROWAVE AND ULTRASOUND MEDIATED ORGANIC SYNTHESIS

Microwave assisted reactions, Microwave activation – advantage of microwave exposure – specific effects of microwave – Neat reactions – solid supportedreactions _ Functional group transformations – condensation reactions – oxidation – reduction reactions – multi-component reactions.

Ultrasound assisted reactions, ultrasound for waste water treatment, cleaning and organic synthesis– oxidation– reduction reactions.

UNIT-III WATER TREATMENT

Sources of water – Quality characteristics of water: total acidity and alkalinity, hardness of water – methods of determination of hardness, total solids, disadvantages of using hard water.

Softening of water: Desalination, Clark‟s process, lime-soda process, ion-exchange process; demineralization of water - Treatment of water: sterilization, flocculation, Industrial treatment – Treatment of wastes or effluents with organic and inorganic

impurities, sewage and sewage treatment; Biochemical oxygen demand (BOD), chemical oxygen demand (COD)

UNIT IV: PLASTICS

Thermosetting and thermoplastics- Effect of polymer structure on properties.

Formation of plastics: copolymerization–properties and uses of plastics-Manufacture by molding process-Commercial resins and plastics: bakelite, urea-formaldehyde, melamine-formaldehyde, epoxy, acrylic and silicon resins, polythene, PVA, PVC, cellulose, cellulose nitrate and acetate.
Disposing of plastics: incineration, biodegradation, recycling and source reduction.

UNIT-V NEW ENERGY SOURCES FOR NEW CENTURY

Renewable energy sources-Introduction to solar energy-Biomass conversion-Sea wave energy-tidal energy-geo-thermal energy-wind energy-nuclear fusion energy. Splitting of water-hydrogen from sunlight-hydrogen economy. Fuel cells-batteries-photovoltaic cells. Nuclear energy-Nuclear fission and fusion-Production of electricity by nuclear reactor-radioactivity and hazards of radioactivity-living with nuclear power-Management of radioactive waste.

Reference Books

1. Environmental Pollution, A.K. De
2. Mike Lancaster , Green Chemistry and Introductory text, II Edition
3. P.T.Anastas and J.C Warner,Green Chemistry theory and Practice, Oxford University press, Oxford (1988).
4. V.K. Ahluwalia, Methods and Reagents of Green Chemistry: An Introduction by Green Chemistry, Ane Books India, 2006.
5. Green Chemistry – Environment friendly alternatives- edited by Rashmi Sanghi& M. M. Srivastava, Narora Publishing House, (2003).
6. Engineering Chemistry- Jain and Jain.
7. Engineering Chemistry- R.K. Sharma.

ELECTIVE-3B SURFACE ANALYTICAL TECHNIQUES & SENSORS

Paper Code: MDCH34B

Course Objectives:

After this course the student should be able

- To understand the principles of ECSA, SERS and other techniques.
- To know the principles and application of electroanalytical techniques.
- To apply the student knowledge in the importance of sensor.
- To make the student knowledgeable in the application of biosensors.

Course Out comes: After studying this course the students will be able to:

CO 1: To understand the principles of ECSA, SERS and other techniques

CO2: To know the principles and application of electro analytical techniques

CO3: To apply the student knowledge in the importance of sensor

CO4: To make the students knowledgeable in the application of biosensors

CO5: The students to gain the knowledge in Electrochemical sensors and Biosensors.

UNIT-I SURFACE ANALYTICAL TECHNIQUES-1

Electron Spectroscopy for Chemical Analysis (ESCA): Principles, Instrumentation, and Analytical Applications. Auger electron spectroscopy: Principles, Instrumentation, Applications. Secondary ion mass spectrometry (SIMS):Principles, Instrumentation, Applications.

Surface enhanced Raman Spectroscopy (SERS): Principles, Instrumentation, Nanoparticulate SERS substrates, Surface enhanced resonance Raman scattering (SERRS), SERRS of Ag and Au metal colloids, Thin solid films, Langmuir-Blodgett Monolayers.

UNIT-II SURFACE ANALYTICAL TECHNIQUES-2

Mapping and imaging, Applications. Electron Energy Loss Spectroscopy (EELS): Principles, Instrumentation, Applications. Electron Microprobe analysis: Principles, Instrumentation, Analysis of semiconductors and crystalline materials, Applications. Low Energy Ion Scattering Spectroscopy: Principle, Instrumentation, Surface structural analysis.

UNIT-III CHEMICAL SENSORS

Importance of Sensors, Biomolecular recognition elements, Artificial molecular-recognition materials, Molecular imprinted polymers, Electrode modification. Fluorescence, chemi and bio-luminescence sensors, Fluorescent tag molecules, Applications.

UNIT-IV ELECTROCHEMICAL SENSORS

Conductometric sensors, Coulometric sensors, Voltammetric sensors, Applications, Neurotransmitters, Amperometric sensors, Chronoamperometric analysis, Multichannel sensors, Microelectrode sensors, Electrochemical Impedance Sensors, Quartz crystal nanobalance sensors.

UNIT-V BIOSENSORS

Molecular recognition, Applications. Surface Plasmon resonance based sensors, Fiber optic sensors, Two dimensional microarray based sensors, Applications for Food Safety – Mycotoxins, adultrants, Biomedical diagnosis
– Cancer markers.

Reference Books

1. Brian R. Eggins, Chemical Sensors and Biosensors, Analytical Techniques in the Sciences (ANTS), 2nd Edition, Wiley, 2002.
2. Gabor Harsanyi, Sensors in Biomedical Applications – Fundamentals, Technology and Applications, CRC Press, 2000.
3. Raluca-Ioana Stefan, Electrochemical Sensors in Bioanalysis, CRC Press, 2001.
4. D J O'Connor, Brett A Sexton, Roger S C Smart (Eds), Surface Analysis Methods in Materials Science, 2nd Edition, Springer, 2010.
5. John C Vikerman, Ian Gilmore (Eds.), Surface Analysis: The Principal Techniques, 2nd Edition, Wiley, 2009.
6. John F Watts, John Wolstenholme, An Introduction to Surface Analysis by XPS and AES, 2nd Edition, Wiley VCH, 2011.

ELECTIVE-3C COMPUTATIONAL METHODS IN CHEMISTRY AND CHEMOMETRICS

Paper Code: MDCH34C

Course Objectives:

After this course the student should be able

- To understand the basic knowledge of use of computer in chemistry.
- To know the software use in drawing the chemical structures.
- To apply the student knowledge in chemometrics.
- To make the student knowledgeable in the application of numerical methods of analysis.

Course Out comes: After studying this course the students will be able to:

CO 1: To understand the basic knowledge of use of computer in chemistry.

CO2: To know the software use in drawing the chemical structures.

CO3: To apply the students knowledgeable in the application of mumerical methods of analysis.

CO4: To apply the student knowledge in chemometrics.

CO5: The students to gain the knowledge in computational methods in chemistry and chemometrics

UNIT-I COMPUTER BASICS

Windows and Linux; MSOFFICE; Statistical Data Processing and Curve Fitting by EXCEL, GRAPHER, SURFER and MATHEMATICA; Chemical Structure Drawing by ISIS Draw, CHEMWIND, ACD Labs and CHEMDRAW; Molecular Modeling by ACD Labs, PCWIN and CHEM 3D; Chemical Databases; Animations and Virtual Chemical Experiments

UNIT-II FORTRAN 77

Types of Constants and Variables in Fortran, Dimension, Data, Type, COMMON and EQUIVALENCE statements, Arithmetic and Logical IF, IF-THEN ELSE Constructs, DO statement, Various types of I/O statements, Library functions, Statement functions, Function subprograms and subroutine subprograms with suitable examples.

UNIT-III NUMERICAL METHODS

Roots of Polynomials, Solution of Linear simultaneous equations, matrix multiplication and inversion. Numerical integration. Statistical treatment of data, variance and correlations, Least square curve fitting.

UNIT-IV COMPUTER APPLICATION

Role of computer in research, data organization, software selection and its applications, solving problems by using scientific software & tools, sample programmes for analysis of data.
Computer Searches of Literature: ASAP Alerts, CA Alerts, SciFinder, ChemPort, ScienceDirect , STN International-Journal home pages.

UNIT-V CHEMOMETRICS

Introduction to Chemometrics, principles of experimental design, factorial and fractional factorial design, specific applications. Response surface methodology and Optimization, Response surface designs, Sequential optimization, specific, numerical problems. Modelling and Knowledge processing: multiple linear regressions, test parameter estimation, PCR PLS, PCA etc. Cluster analysis and descriminant analysis, 46odeling of multiway regression.

Reference Books

1. V. Rajaraman, Fortran 77, Prentice Hall (India), New Delhi.
2. S.D. Conte and C. deBoor, Elementary Numerical Analysis, McGraw-Hill (Intl. Edition) (1987).
3. K. V. Raman, Computers in Chemistry, Tata McGraw Hill (1993).
4. E. Morgan, Chemometrics: Experimental Design, John Wiley & Sons, 2008.

2. Otto Mattias, Chemometrics: Statistics and Computer Application in Analytical Chemistry, Wiley, 2007
3. J.N. Miller and J. C. Miller, Statistics and Chemometrics for Analytical Chemistry, Pearson Prentice Hall, 6th Edition, 2010.
4. Brereton, R.G, Chemometrics: Data Analysis for the Laboratory and Chemical Part, Wiley, 2003.

PRACTICAL-7 ORGANIC CHEMISTRY PRACTICAL- III

Paper Code: MDCH35

Course Objectives:

- To understand the separations techniques.

Course Out comes: After studying this course the students will be able to:

CO 1: To understand the Column, Paper, Thin Layer Chromatography.

CO2: To know about the High Performance Thin Layer Chromatography.

CO3: To familiarize the two dimensional Paper Chromatography, Reverse phase paper chomatography.

CO4: To learn about the Gas-liquid Chromatography.

CO5: To know about the High Performance Liquid chromatography.

Chromatographic Separations

Column chromatography - separation of anthracene and picric acid from anthracene picrate.
Thin layer chromatography separation of green leaf pigments.
Paper chromatography-Identification of amino acid.

Any FOUR Estimations

Estimation of aniline
Estimation of phenol
Estimation of glucose
Estimation of amino group
Estimation of amide group
Saponification of fat or an oil
Iodine value of an oil
Estimation of sulphur in an organic compound
Estimation of methyl ketone

Special Interpretation Of Organic Compounds- IR, NMR and MASS Spectra of the following types of compounds

1. Alcohls (primary, secondary and tertiary)
2. Aldehydes
3. Ketones
4. Mono &dihalo compounds
5. Amines
6. Esters
7. Amides
8. Alkenes and alkynes

Reference Books

1. Arthur I.Vogel, A text book of Practical Organic Chemistry, ELBS
2. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern limited.
3. N.N. Greenwood and A. Earnshaw, Chemistry of the Elements, Vol.II, Pergamon Press (1997).
4. R. M. Silverstein, F. X. Webster, D. J. Kiemle. Spectrometric Identification of Organic Compounds, Seventh Edition.

PRACTICAL-8 **INORGANIC CHEMISTRY PRACTICAL – III**

Paper Code: MDCH36

Course Objectives:

- To understand the spectral techniques.

Course Out comes: After studying this course the students will be able to:

CO 1: To get the basic knowledge of Spectra techniques of inorganic complexes.

CO2: To estimation of various Inorganic Complexes

CO3: Understand the concepts of Alloys and ores.

CO4: To determine the composition of Alloys.

CO5: Understand the Physical and Chemical properties of Ores.

Analysis of Alloys

Estimation of tin and lead in solder.
Estimation of copper and zinc in brass/Bronze.
Estimation of chromium and nickel in stainless steel.

Analysis of Ores

Dolomite, Galena, Pyrolusite, Copper pyrites

Quantitative Analysis

Quantitative analysis of mixtures of iron –magnesium; iron – nickel; copper – nickel and copper – zinc.

List of Spectra to be given for interpretation.

$_{31}P$ NMR Spectra of methylphosphate

^{31}P NMR Spectra of HPF_2

^{19}F NMR Spectra of CIF_3

$_1H$ NMR Spectra of Tris (ethylthioacetanato) cobalt (III)

Explain high resolution $_1H$ NMR spectra of (N-propylisonitrosoacetylacetoneuninato) (acetylacetonato) Nickel (II) ESR

Spectra of the aqueous $ON(SO_3)_{2-}$ ion.

ESR Spectra of the H atoms in CaF_2.

ESR Spectra of the $[Mn(H_2O)_6]^{2+}$.

ESR Spectra of the bis (salicylaldiminato) copper (II)

IR Spectra of the sulphato ligand.

IR Spectra of the dimethylglyoxime ligand and its Nickel (II) complex. IR Spectra of carbonyls

Mossbauer spectra of $FeSO_4.7H_2O$

Mossbauer spectra of $FeCl_3$.

Mossbauer spectra of$[Fe(CN)_6]^{3-}$

Mossbauer spectra of $[Fe(CN)_6]^{4-}$

PRACTICAL-9 **PHYSICAL CHEMISTRY PRACTICAL – III**

Paper Code: MDCH37

Course Objectives:

- To understand the instruments techniques**.**

Course Out comes: After studying this course the students will be able to:

CO 1: Potentiometric titration of a mixture of acids.

CO2: Precipitation titrations -$AgNO_3$ vs KCl

CO3: Determination of pH and calculation of pKa.

CO4: Determination of Strength of KI using potentiometric titration between FAS and KI.

CO5: To get Knowledge of Various pH and Potentiometric titrations**.**

Conductometric/Potentiometric Titrations-II:

1. Determination of the equivalent conductance of a weak acid at different concentrations and verify Ostwald's dilution law and calculate the dissociation constant of the acid.
2. Determination of equivalent conductance of a strong electrolyte at different concentrations and examine the validity of the Onsager's theory as limiting law at high dilutions.
3. Determination of equivalent conductance of a strong electrolyte and verification of Debye-Huckel-Onsager Equation
4. Verification of Ostwald's Dilution law for a weak electrolyte.
5. Determination of pH and calculation of pKa.
6. Determination of strength of KI using potentiometric titration between FAS and KI.
7. Determination of strength of FAS using potentiometric titration between $KMnO_4$ and FAS.
8. Experiment on precipitation titration of mixture of halides by EMF measurements.

Spectral Interpretation:

Experiments given only to familiarize the interpretation of spectra provided. Interpretation of simple UV-Visible spectra of simple molecules for the calculation of molecular data and identification of functional groups (5 typical spectra will be provided).
IR and NMR spectral calculations of force constant – identification and interpretation of a spectra (5 each in IR and NMR will be provided).

Reference Books

1. Findlay's practical Physical Chemistry, Revised and edited by B.P. Levitt, 9th edn.,Longman, London, 1985.
2. J.N. Gurtur and R. Kapoor, "Advanced Experimental Chemistry," Vol. I, S.Chand & Co., Ltd., New Delhi.
3. Practical Physical Chemistry by B. Viswanathan and P.S. Raghavan, Viva publishers.

SEMESTER-IV

CORE-10 **ORGANIC CHEMISTRY –IV**
(ADVANCED ORGANIC CHEMISTRY)

Paper Code: MDCH41

Objectives:

- To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis. To learn retrosynthetic approach towards organic synthesis.
- At the end of the course, the learners should be able to use various reagents and organic reactions in a logical manner in organic synthesis.
- Learnt the basic principles of photochemistry and pericyclic reactions.

Course Out comes: After studying this course the students will be able to:

CO 1: To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis in synthetic methodology.

CO2: To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis. To learn retro synthetic approach towards organic synthesis.

CO3: This unit clarifies the plain theories of three and four membered heterocyclic reactions in organic synthesis. Students will advantage information on reaction mechanism.

CO4: On this unit conclusion of the progress the students should have Absorb photochemical reactions also study in the course.

CO5: On this unit conclusion of the progress the students should have Absorb the pericyclic reactions of ring opening and ring close electrochemical and photochemical reactions also study in the course

UNIT-I SYNTHETIC METHODOLOGY

An introduction to synthons and synthetic equivalents, functional group interconversions, Planning and execution of multistep synthesis- overall calculation for multistep synthesis- synthesis of simple molecules. The importance of the order of events in organic synthesis, One group C-C disconnections – Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, Olefination of carbonyl compounds, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polaritiy, cyclization reactions, amine synthesis.

UNIT-II MODERN SYNTHETIC METHODS

Modern Synthetic Methods: Baylis-Hillman reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Brook rearrangement. Palladium mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira coupling reactions. Stereoselective synthesis of tri- and tetra-substituted olefins, Synthetic applications of Claisen rearrangement.

UNIT-III CONSTRUCTION OF RING SYSTEMS

Construction of Ring Systems: Different approaches towards the synthesis of three, four, five, and six-membered rings. Pauson-Khand reaction, Bergman cyclization; Nazarov cyclization, inter-conversion of ring systems (contraction and expansion). Construction of macrocyclic rings and ring closing metathesis.

UNIT-IV PHOTOCHEMISTRY

Organic photochemistry – fundamental concepts –Joblonski diagram -energy transfer –characteristics of photoreactions – photoreduction and photooxidation, photosensitization. Photoreactions of ketones and enones – Norrish Type I and II reactions – Paterno-Buchi reaction – photo-Fries rearrangement – photochemistry of alkenes, dienes and aromatic compounds – di-π-methane rearrangement. Photochemistry of α,β-unsaturated carbonyl compounds – photolytic cycloadditions and photolytic rearrangements – photo additions – Barton reaction.

UNIT- V PERICYCLIC REACTIONS

Pericyclic Analysis of electrocyclic, cyclo addition and sigmatropic reactions – correlation diagrams for butadiene – cyclobutene system, hexatriene systems. FMO and PMO approach, electrocyclic reactions, - conrotatory and dis rotatary motions, 4n , 4n+2 and allyl systems. Sigmatropic rearrangement, supra and antarafacial shifts of H. Sigmatropic shifts involving carbon moieties, 3,3- and 5,5-sigmatropic rearrangement – Cope and Claisen rearrangement.

Reference Books

1. R.O.C. Norman, Principles of Organic Synthesis, Second edn., Chapman and Hall, 1993.
2. R.K. Mackie, D. M.Smith and R.A. Aatkin, Guide Book to Organic Synthesis, 2ndedn. Longman Scientific and Technical, London, 1990
3. S.Warren, Designing Organic Synthesis – A Programmed Introduction to Synthon Approach, Wiley, NY, 1978
4. R.O.C. Norman, Principles of Organic Synthesis, II Edn., Chapman and Hall, 1993.
5. Jaya singh and Jagadhambasingh, Photochemistry and Pericyclic reactions, New Age international Publishers, New Delhi, 2010.
6. N.J.Turro, Modern Molecular Photochemistry, Benjamin, Cumming, Menlo Park, California.
7. K.K.Rohatgi, Mukherjee, Fundamentals of Photochemistry, New Age International Pvt. Ltd, Chennai, 2009.
8. R.P.Wayne, Photochemistry, Butterworths, London.

CORE-11 SCIENTIFIC RESEARCH METHODOLOGY

Paper Code: MDCH42

Objectives:

- To study about the importance of research, literature survey, error analysis, statistical treatment.
- To know the various indexes and abstracts in science and technology as a source of in format ion in chemistry.
- To study about the conventions of writing thesis.

Course Out comes: After studying this course the students will be able to:

CO 1: To study about the importance of research, literature survey, error analysis, statistical treatment.

CO2: To know the various indexes in science and technology as a source of in format ion in chemistry.

CO3: To know the various abstracts in science and technology as a source of in format ion in chemistry.

CO4: To student about the conventions of writing thesis.

CO5: Drafting of research reports efficiently

UNIT-I MEANING OF RESEARCH

Nature and importance of research-aims, objective, principles and problems-selection of research problems, purpose of research, scientific method, role of theory, characteristics of research. Types of research: fundamental or pure research, applied research, action research, historical research, experimental research.

UNIT-II CHEMICAL LITERATURE

Sources of chemical information: primary, secondary and tertiary sources.
Indexes and abstracts in science and technology: applied science and technology index, chemical abstracts, chemical titles, current chemical reactions, current contents, physics abstracts, science citation index. Beilstein compilations of data, synthetic methods and techniques, treatises, reviews.

UNIT-III CHEMICAL ABSTRACTS

Current awareness searching: Mission and history-CA weekly issues, CA issue indexes. Retrospect ive searching: CA volume indexes-general subject index, chemical substance index, formula index, index of ring systems, author index, patent index. CA Collective indexes: Collective index (CI), decennial index (DI).

UNIT-IV SCIENTIFIC WRITING

Scientific writings: research reports, theses, journal articles, and books. Steps to publishing a scientific article in a journal: types of publications communications, articles, reviews; when to publish, where to publish, specific format required for submission, organization of the material. Documenting: abstracts-indicative or descriptive abstract , informative abstract, footnotes, end notes, referencing styles, bibliography-journal abbreviations.

UNIT-V COMPUTER SEARCHES OF LITERATURE

ASAP Alerts, CA Alerts, SciFinder, ChemPort, ScienceDirect, Web of science, Scopus, STN International.

Reference Books

1. R. L. Dominoswki, Research Methods, Prentice Hall, 1981.
2. J. W.Best, Research in Education, 4th ed. Prentice Hall of India, New Delhi, 1981.
3. H. F. Ebel, C. Bliefert and W. E. Russey, The Art of Scientific Writing, VCH, Weinheim, 1988.
4. B. E. Cain, The Basis of Technical Communicating, ACS., Washington, D.C., 1988.
5. H. M. Kanare, Writing the Laboratory Notebook; American Chemical Society: Washington, DC, 1985.
6. J. S. Dodd, Ed., The ACS Style Guide: A Manual for Authors and Editors; American Chemical Society: Washington, DC,1985.
7. Gibaldi, J. Achtert, W. S. Handbook for writers of Research Papers; 2nd ed.; Wiley Eastern, 1987.
8. Joseph, A. Methodology for Research; Theological Publications: Bangalore, 1986.

ELECTIVE-4A **APPLICATION OF SPECTRAL TECHNIQUES TO INORGANIC COMPOUNDS**

Paper Code: MDCH43A

Objectives:

- On the completion the course the students will have the knowledge of applications of various spectral techniques to inorganic compounds.

Course Out comes: After studying this course the students will be able to:

CO 1: Know the basic concepts of various spectroscopies. (NMR, ESR, IR AND MOSSBAUER)

CO2: Understand the various Spectroscopic methods.

CO3: Ability to apply the basic principles of various spectroscopic, electro and thermo analytical methods to characterize the compounds.

CO4: Acquire skill to Interpret the spectra for Inorganic compounds

CO5: To get the knowledge and applications of various spectral techniques to inorganic compounds.

UNIT-I ELECTRONIC SPECTROSCOPY

Terms and states of d_n ions- electronic spectra of coordination compounds - selection rules – Orgel and Tanabe-Sugano diagram for transition metal complexes. Charge transfer spectra.

UNIT-II INFRARED AND RAMAN SPECTROSCOPY

IR spectroscopy-principle-fundamental modes of vibrations- H_2O, CO2 and SO2- change of IR spectra of ligands upon coordination-urea, thio urea, SO42-, NO3-, nitriles, carboxylate, cyanate and thiocyante anions. Finger print region- IR spectra of metal carbonyls. Effect of isotopic substitution on IR spectra.

Raman spectroscopy-principle-mutual exclusion principle-combined application of IR and Raman to inorganic molecules.

UNIT-III NMR SPECTROSCOPY

Application of NMR ($_{19}F$, $_{31}P$ and $_{13}C$) techniques to characterize the inorganic compounds. Chemical shifts-application of spin-spin coupling to structure determination-H_3PO_3 and H_3PO_2, P_4 S_3, BrF_5,- applications involving magnitude of coupling constants-consequences of nuclei with quadrupole moments-NMR shifts of paramagnetic complexes-Contact shifts-spectrum of $P_3N_3Cl_4F_2$, $P_4N_4Cl_6$.

UNIT-IV EPR SPECTROSCOPY

Theory of EPR spectroscopy - Spin densities and McConnell relationship – Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy – Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions.

UNIT-V MOSSBAUER SPECTROSCOPY

Principle-Isomer shifts – Magnetic interactions – Mossbauer emission spectroscopy – application to low and high spin iron and tin compounds.

Reference Books

1. R.S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern Company .
2. F.A. Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 3rd ed., Wiley-Eastern Company, New Delhi 1990.
3. P.J. Wheatley, The Determination of Molecular Structure, .
4. Lewis and Wilkins, Modern Coordination Chemistry,.
5. E.A.V.Ebsworth, Structural Methods in Inorganic Chemistry, 3rd ed., ELBS, Great Britain, 1987.

ELECTIVE-4B INSTRUMENTAL METHODS OF ANALYSIS

Paper Code: MDCH43B

Objectives:

On the completion the course the students will have the knowledge of
- Various instrumental techniques.
- The students should have learnt data analysis and electro analytical techniques.

Course Out comes: After studying this course the students will be able to:

CO 1: The students will have the knowledge of various instrumentational Techniques.

CO2: The students to get the knowledge of mean, median, precision and accuracy in chemical analysis.

CO3: The students to get their knowledge in absorption spectrometry, Flame photometry, Infra-red and Raman spectroscopy.

CO4: The students to get their knowledge in NMR, ESR and Mossbauer spectroscopy

CO5: To understand the synthesis of organic and inorganic compounds by irradiation, radiometric analysis and radiography.

UNIT–I DATA ANALYSIS

Definition of Terms – Mean, Median, Precision and accuracy; Errors in chemical analysis- systematic errors and random errors. Treatment of data – Basic statistical concepts and frequency distribution, Average and measure of dispersion; Significance of Gaussian distribution curves; Null hypothesis; confidence interval of mean, Criteria for rejection of data; Regression and correlation; quality control and control chart.

UNIT–II OPTICAL METHODS OF ANALYSIS

Absorption spectrometry – Beer Lamberts law; Spectrophotometry: UV visible spectroscopy- photometric titrations; Fluorimetry, turbidimetry and nephelometry.

Flame Photometry–Theory, instrumentation and a few important applications; Atomic absorption spectroscopy (AAS) – Theory, instrumentation and applications; Atomic fluorescence.

Infra-red spectroscopy – Theory and instrumentation – source, monochromators, detectors; dispersive and non dispersive instruments; sample handling techniques; qualitative analysis and quantitative applications.

Raman spectroscopy – Theory, instrumentation – source of radiation and detectors; few qualitative and quantitative applications; Resonance Raman spectroscopy.

UNIT–III NMR, ESR AND MOSSBAUER SPECTROSCOPY

Nuclear Magnetic Resonance Spectroscopy –Theory, relaxation and saturation processes, Environmental effects; instrumentation – type of magnets, source, detector and sample handling; few application of proton NMR; qualitative and quantitative analysis.

Electron Spin Resonance –Theory, instrumentation and a few applications in qualitative and quantitative analyses.

Massbauer spectroscopy: principle, instrumentation – applications; molecular structure, isomerism, electronic structure.

UNIT–IV POLAROGRAPHY, AMPEROMETRY AND CHROMATGRAPHY

Polarography – Theory, apparatus, DME, diffusion kinetic catalytic currents, current voltage curves for reversible and irreversible system, qualitative and quantitative application to inorganic systems.

Amperometric titrations – Theory, apparatus, types of titration curves, successive titrations and two indicator electrodes-applications.

TLC, Colum, gas, ion exchange, Gel permeation, Gas liquid chromatography-principle, retention time values, instrumentation, carrier gas, column, detectors-thermal conductivity, flame ionization and electron capture; few applications of GLC.

UNIT–V RADIOCHEMICAL METHODS

Hot atom chemistry – the Szilard – chalmers process, chemistry of recoil atoms, chemical effects no radiative decay, solvated electron. Uses of radiations in the study of matter, neutron activation analysis, dilution analysis, dosimetry, synthesis of organic and inorganic compounds by irradiation, radiometric analysis, radiography.

Reference Books

1. Willard, Merit, Dean and Settle, Instrumental Methods of Analysis,
2. Schoog, Holler, Nieman, Principles of Instrumental Analysis**,** Thomson Asia Pte Ltd., Singapore, 2004.
3. D.A.Skoog and D.M.West Fundamentals of Analytical Chemistry, Holt Rinehart and Winston Publications, IV Edn, 2004.
4. W. Kemp, NMR in Chemistry, MacMillan Ltd,1986.

ELECTIVE-4C ENVIRONMENTAL CHEMISTRY

Paper Code: MDCH43C

Objectives:

After this course the student should be able

- To understand the basic knowledge of natural cycles in the environment.
- To know the various pollutants affecting environment.
- To apply the student knowledge in preventing pollution.

Course Out comes: After studying this course the students will be able to:

CO 1: To understand the Environment terminology and nomenclatures

CO2: To know the earth radiation balance and radical in the atmosphere

CO3: To understand the soil properties and acid base and ion exchange reaction in Soil.

CO4: To understand concept of the aerosols, photochemical smog and acid rain.

CO5: To know the water quality parameters such as dissolved oxygen, BOD, COD, Total organic carbon and chlorides.

UNIT-I INTRODUCTION TO ENVIRONMENTAL CHEMISTRY

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, The natural cycles of environment (Hydrological, Oxygen, Nitrogen, Phosphorous and Sulphur cycles).

UNIT-II ATMOSPHERE

Regions of the atmosphere, Reactions in atmospheric chemistry, Earth's radiation balance, Particles, ion and radicals in the atmosphere, stratospheric chemistry: The chemistry of ozone layer, The role of chemicals in ozone destruction, The green-house effect and Global warming, El-Nino phenomenon.

UNIT-III LITHOSPHERE

The terrestrial environment, Soil formations, Soil properties (physical/chemical), inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil, waste and pollutants in soil, waste classification and disposal.

UNIT-IV AIR POLLUTION

Air pollutants (sources, classification, sampling and monitoring): Particulates, Aerosols, SO_X, NO_X, CO_X and hydrocarbon emission, Photochemical smog, Autoexhausts, Acid-rains, Air-quality standards. Method of control of air pollution: Method of control of air pollution, electrostatic precipitation wet & dries scrubber, filters, gravity and cyclonic separation, Adsorption, absorption and condensation of gaseous effluent.

UNIT-V WATER POLLUTION

Water pollutants (sources, sampling and monitoring), Water-quality parameters

and standards: physical and chemical parameters (colour, odour, taste and turbidity), Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation. Method of control of water pollution: Water and waste water treatment, aerobic and anaerobic, aeration of water, principle of coagulation, flocculation, softening, disinfection, demineralization and fluoridation.

Reference Books

1. G.W. Vanloon, S.J. Duffer, Environmental Chemistry – A Global Perspective, (2000) Oxford University Press.
2. F.W. Fifield and W.P.J. Hairens, Environmental Analytical Chemistry, 2nd Edition (2000), Black Well Science Ltd.)
3. Colin Baird, Environmental Chemistry, (1995) W.H. Freeman and Company, New York.
4. A.K. De, Environmental Chemistry, 4th Edition (2000), New Age International Private Ltd., New Delhi.
5. Peter O. Warner, Analysis of Air Pollutants,1st Edition (1996), John Wiley, New York.
6. S.M. Khopkar, Environmental Pollution Analysis, 1st Edition (1993), Wiley Estern Ltd., New Delhi.
7. S.K. Banerji, Environmental Chemistry, 1st Edition (1993), Prentice-Hall of India, New Delhi.

CORE-12 **PROJECT**

Paper Code: MDCH44

Course Objectives:

- To understand how do to the project**.**

Course Out comes: After studying this course the students will be able to:

CO 1: Identify the research problems.

CO2: Analysis of data using chem software.

CO3: Drafting of research reports efficiently.

CO4: To know the various indexes and abstracts in science and technology as a source of in format ion in chemistry.

CO5: To study about the conventions of writing thesis**.**

Field of Project – Organic / Inorganic / Physical Chemistry

No. of hours/week : 18

No. of Credit : 05

Supervisor & research topic:

The guide and area of research should be allotted to each student before the end of third semester. Each guide shall have a maximum of five students.

Plan of Work:

The student should prepare the plan of project work with due consultation of guide and get the approval of the Head of the Department. In case the student wants to avail the facility from other University/laboratory, they will undertake the work with the permission of the guide and acknowledge the facilities utilized by them.

The duration of the dissertation research shall be a minimum of three months in the fourth semester.

Dissertation Work outside the Department:

In case the student stays away for work from the Department for more than one month, specific approval of the Head of the Department should be obtained.

No. of copies of dissertation:

The students should prepare four copies of dissertation and submit the same for the evaluation by Examiners. After evaluation, one copy is to be retained in the Department library and one copy is to be submitted to the University (COE) and one copy each can be held by the guide and student.

Format to be followed:

The format/certificates for dissertation to be submitted by the students are given below:

Format for the preparation of project work:

(a) Title page

(b) Certificate from the guide

(c) Declaration of Student

(d) Acknowledgement

(e) Table of contents

CONTENTS

Chapter No.	TITLE
1.	Introduction
2.	Review of Literature
3.	Materials and Methods
4.	Results and Discussion
5.	Summary
6.	References

Note :

1. Blue colour indicates the syllabus change.
2. Red colour indicates the Job oppournity from various chemical industries

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